



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 11:04 PM UTC

PDB ID : 8WYA / pdb_00008wya
EMDB ID : EMD-37921
Title : Cryo-EM structure of DSR2-tube complex
Authors : Zhang, J.T.; Jia, N.; Liu, X.Y.
Deposited on : 2023-10-30
Resolution : 3.62 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

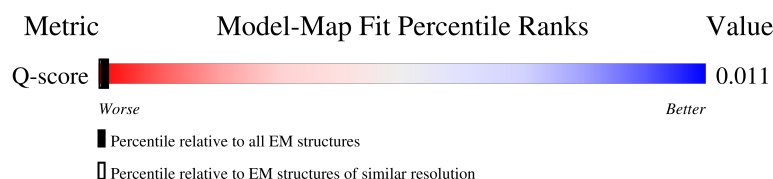
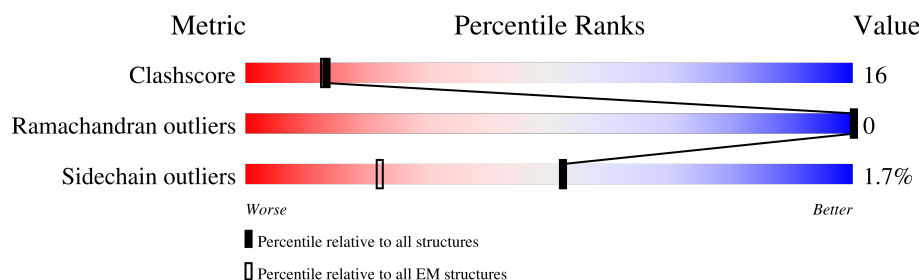
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11773 (3.12 - 4.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1005	47% 57% 34% 9%
1	B	1005	44% 59% 32% 8%
1	D	1005	59% 59% 32% 8%
1	E	1005	60% 62% 28% 9%

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Mol	Chain	Length	Quality of chain
2	C	264	31% 22% 21% 56%
2	F	264	44% 31% 12% 56%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32621 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SIR2 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	915	Total	C	N	O	S	0	0
			7655	4965	1230	1430	30		
1	B	923	Total	C	N	O	S	0	0
			7706	4999	1241	1437	29		
1	D	921	Total	C	N	O	S	0	0
			7705	4995	1241	1439	30		
1	E	919	Total	C	N	O	S	0	0
			7677	4982	1236	1430	29		

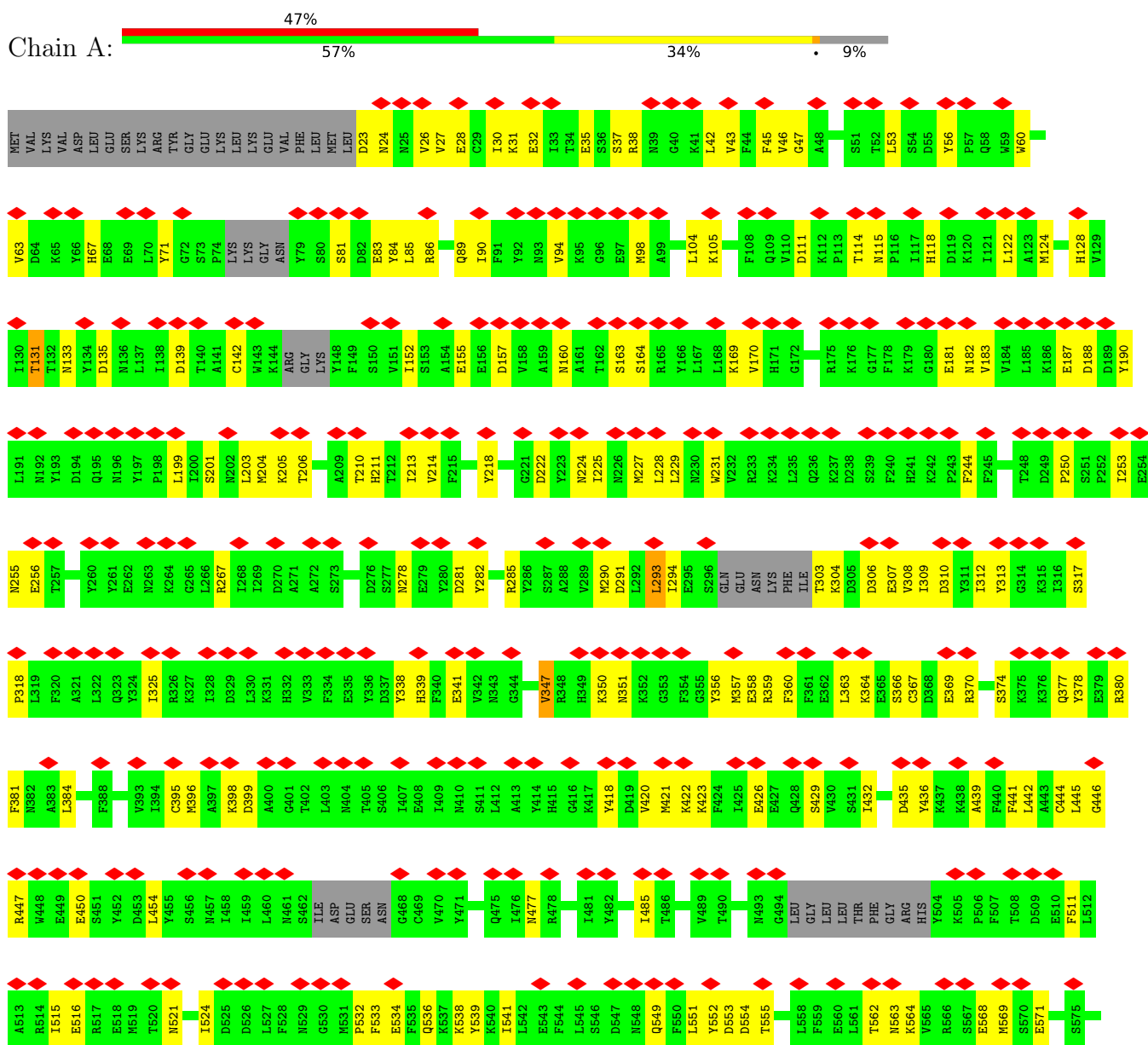
- Molecule 2 is a protein called Bacillus phage SPbeta tube protein.

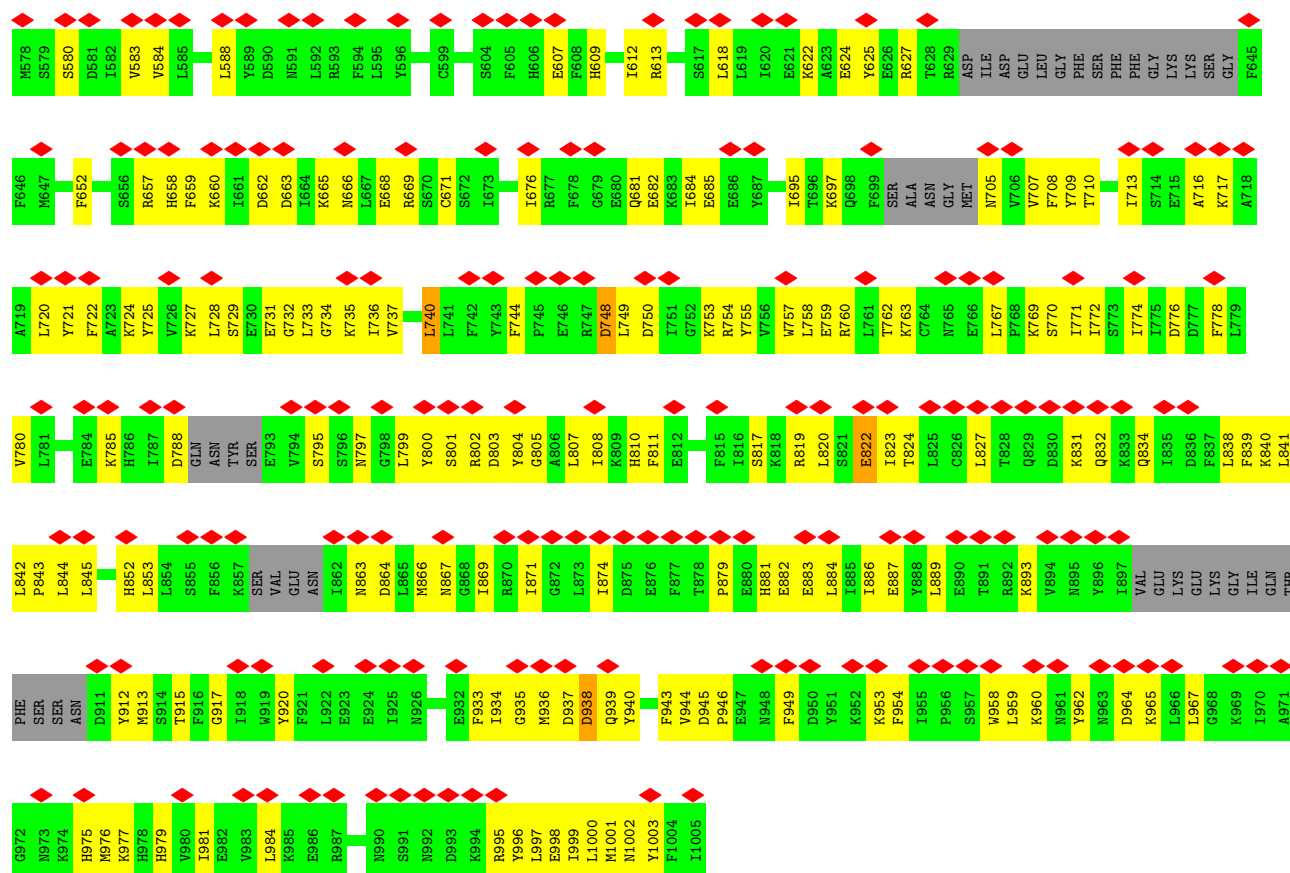
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	116	Total	C	N	O	S	0	0
			939	604	146	186	3		
2	F	116	Total	C	N	O	S	0	0
			939	604	146	186	3		

3 Residue-property plots

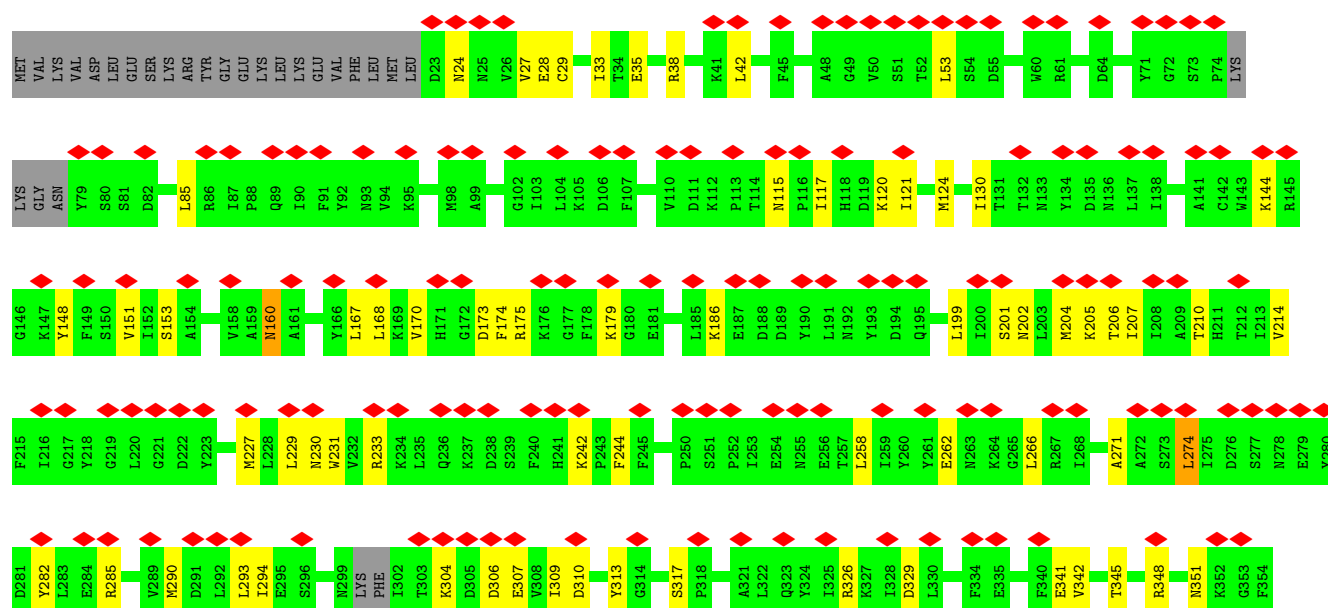
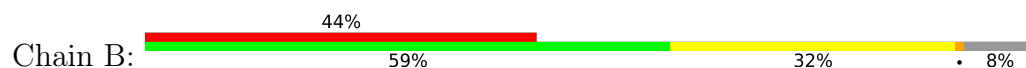
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

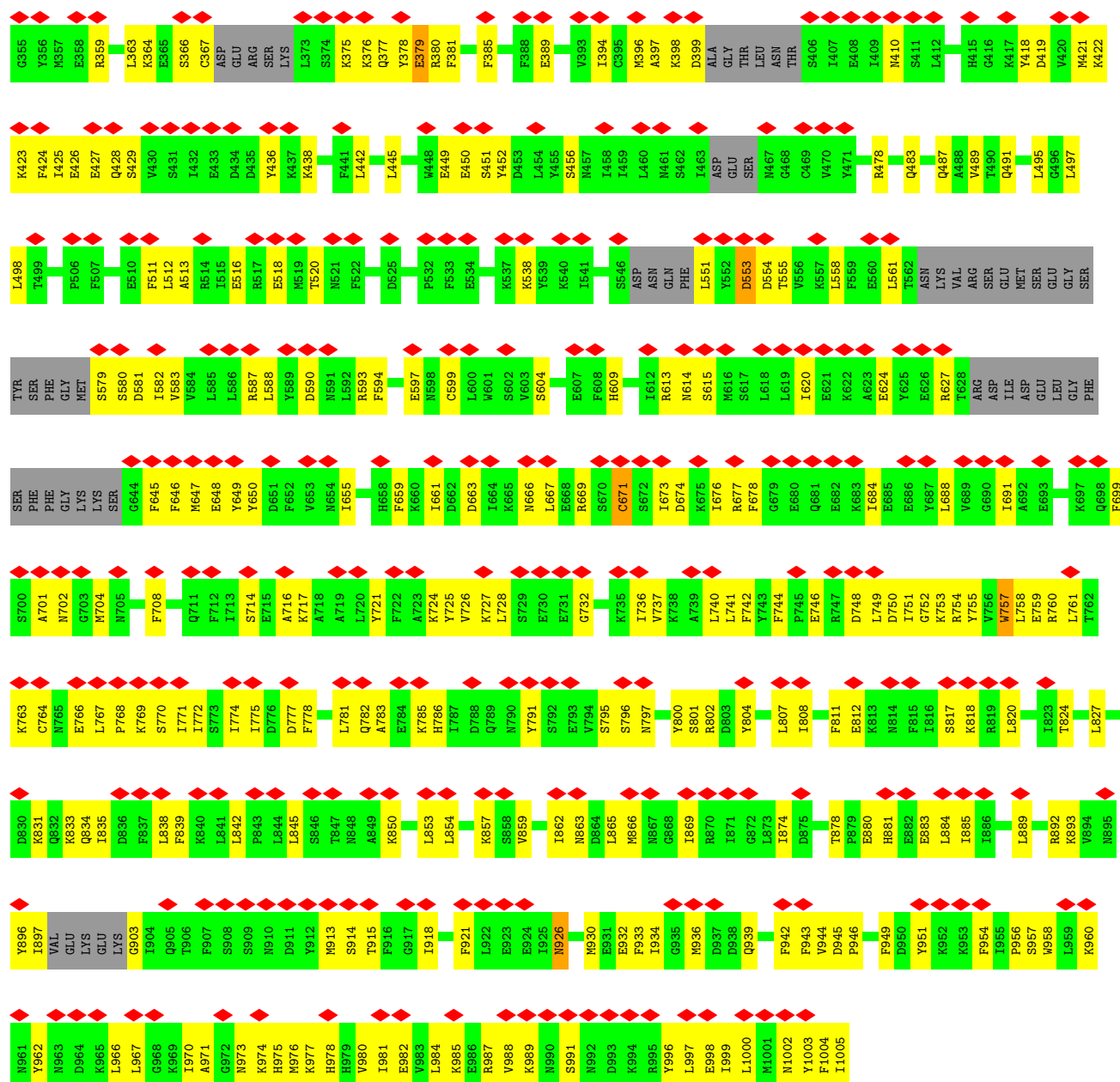
• Molecule 1: SIR2 family protein



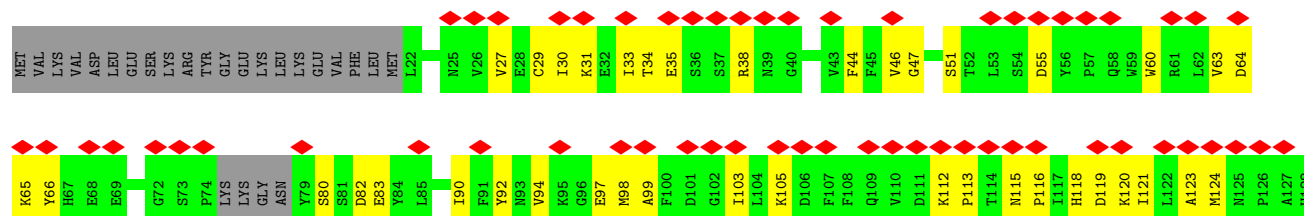


• Molecule 1: SIR2 family protein





• Molecule 1: SIR2 family protein

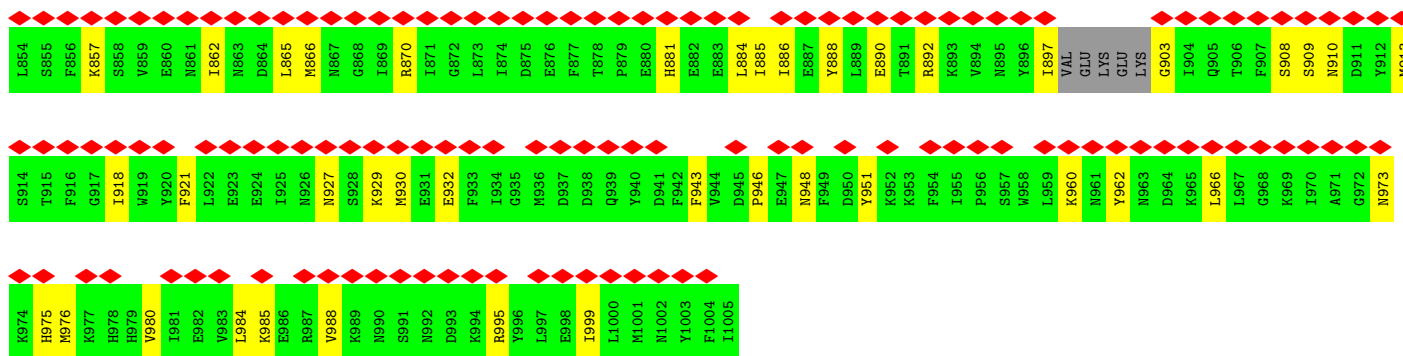


D964	K965	L966	L967	G968	K969	L970	A971	G972	N973	K974	H975	H976	K977	H978	H979	V980	L981	E982	L983	L984	K985	E986	L987	L988	K989	N990	S991	N992	D993	K994	L997	E998	L999	L1000	M1001	N1002	Y1003	F1004	I1005																				
L199	I200	S201	N202	L203	M204	K205	T206	I207	I208	V214	F215	I216	G219	R220	G221	K222	Y223	N224	L228	L229	M230	E231	V232	L235	Q236	P237	PHE	I238	K304	S239	F240	H241	K242	P243	F244	F245	I246	R247	P250	S251	P252	N255	E256	T257	L258	I259	K264	G265	L266	R267	I268	L269	D270	A271					
A272	S273	L274	D275	I276	S277	N278	E279	Y280	D281	Y282	L283	E284	R285	Y286	S287	A288	V289	M290	L291	L292	L293	I294	E295	S296	Q297	E298	ASN	LYS	PHE	ILE	T303	K304	D305	D306	E307	V308	I309	D310	Y311	I312	K315	I316	S317	P318	L319	F320	E321	A322	L322	Q323	Y324	I325	R326	K327	I328	D329	L330	K331	H332
V333	F334	E335	Y336	D337	Y338	H339	F340	E341	V342	N343	G344	T345	V346	R347	H348	K349	K350	N351	K352	G353	F354	G355	Y356	M357	E358	R359	F360	F361	E362	L363	K364	E365	S366	C367	D368	E369	R370	S371	K372	L373	S374	K375	R380	F381	N382	A383	L384	F385	N386	F387	F388	E389	V393	I394	C395	M396	A397		
K398	D399	A400	G401	T402	L403	N404	T405	A406	I407	E408	I409	A413	Y414	H415	G416	K417	Y418	D419	V420	M421	K422	K423	F424	I425	E426	E427	Q428	S429	V430	S431	I432	E433	D434	D435	Y436	F440	F441	L442	A443	C444	L445	G446	R447	W448	E449	E450	S451	Y455	I458	I459	L460	N461	S462	ILE	ASP				
GLU	SER	ASN	G468	C469	Y470	Y472	L473	S474	Q475	I476	N477	R478	Y479	R480	I481	Y482	Q483	S484	T486	Q487	V488	Y489	T490	Q491	F492	M493	G494	LEU	GLY	LEU	LEU	THR	PHE	GLY	ARG	HIS	Y504	K505	P506	F507	T508	D509	E510	F511	L512	A513	R514	I515	E516	R517	E518	M519	T520	N521	F522	N523	I524		
D525	D526	L527	F528	N529	G530	M531	P532	F533	E534	F535	Q536	K537	K538	Y539	K540	I541	L542	E543	F544	L545	S546	D547	N548	Q549	F550	L551	Y552	D553	D554	T555	V556	F559	E560	L561	T562	N563	K564	V565	R566	S567	E568	M569	S570	E571	G572	S573	Y574	S575	F576	G577	M578	S579	S580	D581	I582	V583	V584	L585	
L588	Y589	D590	N591	L592	R593	F594	L595	Y596	E597	L600	H601	H606	E607	Q610	Y611	L612	R613	N614	S615	M616	S617	L618	L619	L620	E621	K622	A623	E624	E625	E626	R627	T628	ASP	ILE	ASP	GLU	LEU	PHE	SER	PHE	GLY	LYS	LYS	ASN	GLY	GLY	F645	F646	H647	V650	D651	F652							
V653	N654	L655	S656	R657	H658	F659	K660	L661	D662	D663	L664	K665	H666	L667	R668	R669	S670	L673	D674	K675	L676	F677	F678	Q681	E682	K683	L684	E685	E686	V687	L688	G689	L691	A692	E693	E694	T695	T696	K697	Q698	F699	SER	ALA	ASN	GLY	GLY	M705	Y709	T710	Q711	F712	L713	S714	E715					
A716	K717	A718	A719	L720	Y721	F722	A723	K724	Y725	V726	L733	G734	K735	I736	Y737	K738	L740	L741	F742	Y743	F744	D748	L749	D750	I751	G752	K753	R754	Y755	V756	W757	L758	E759	R760	L761	T762	K763	C764	N765	E766	L767	P768	K769	S770	I771	I772	S773	I774	I775	D776	F777	F778							
L779	V780	K785	H786	I787	D788	GLN	ASN	TYR	SER	E793	V794	S795	S796	N797	G798	L799	Y800	S801	R802	D803	Y804	G805	A806	G868	L869	R870	H871	G872	L873	I874	D875	E876	F877	T878	R879	E880	H881	E882	E883	L884	I885	I886	E887	Y888	Q829	D830	K831	Q832	K833	Q834	R835	D836	F837	L838	F839	VAL	GLU	LYS	LYS
F843	L844	L845	L846	S846	T847	N848	A849	D911	Y912	H913	F916	G917	F921	L922	E923	E924	I925	N926	D927	L984	K985	S928	R929	M930	E931	E932	F933	G934	L935	G936	D937	E938	Q939	Y940	D941	F942	F943	E944	D945	P946	E947	N948	F949	D950	Y951	K952	K953	F954	I955	P956	S957	W958	L959	K960	N961	Y962	N963		

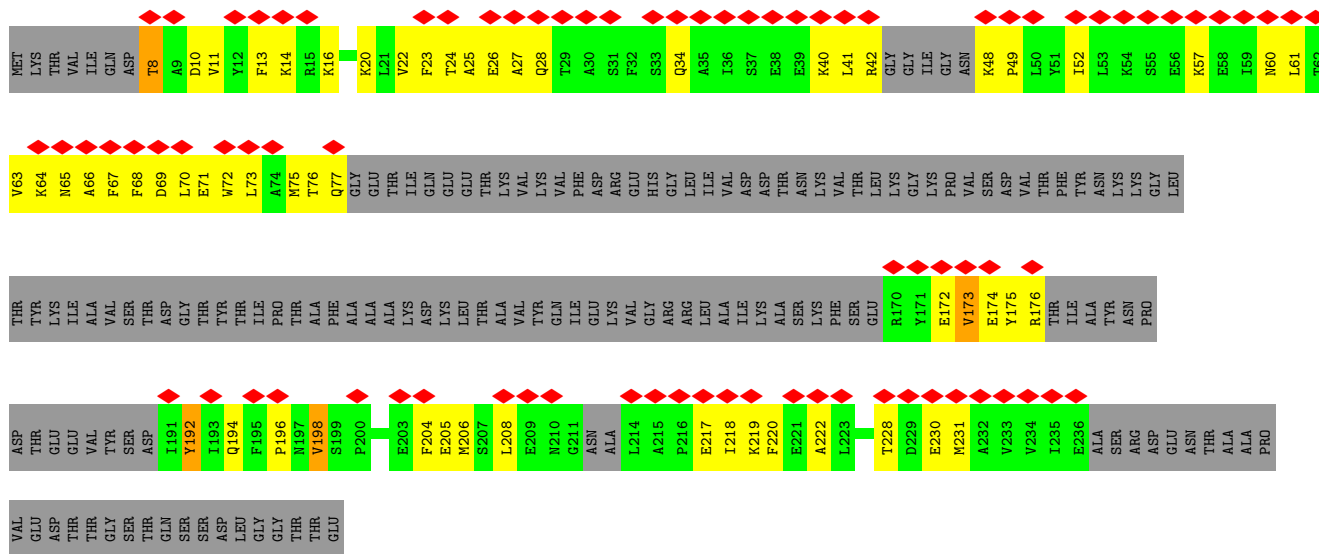
• Molecule 1: SIR2 family protein

Chain E:

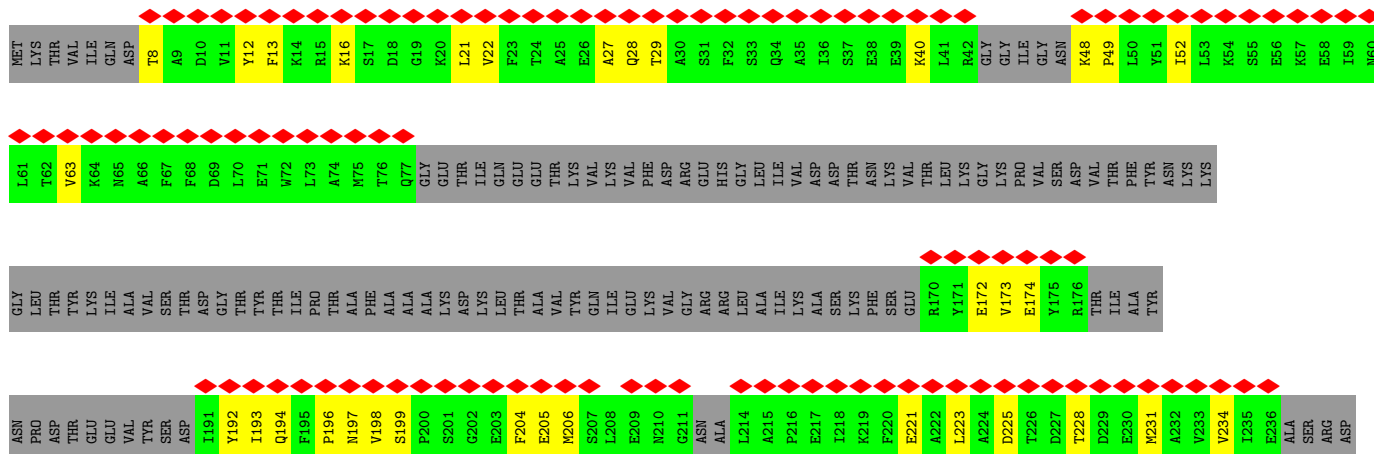
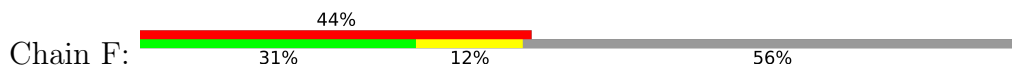




- Molecule 2: Bacillus phage SPbeta tube protein



- Molecule 2: Bacillus phage SPbeta tube protein



GLU
ASN
THR
ALA
ALA
PRO
VAL
GLU
ASP
THR
THR
GLY
SER
THR
GLN
SER
SER
ASP
LEU
GLY
GLY
THR
THR
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16411	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.732	Depositor
Minimum map value	-0.956	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	454.47998, 454.47998, 454.47998	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.988, 0.988, 0.988	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/7829	0.41	0/10541
1	B	0.15	0/7882	0.41	1/10617 (0.0%)
1	D	0.13	0/7880	0.34	0/10609
1	E	0.13	0/7851	0.34	0/10574
2	C	0.20	0/953	0.53	0/1280
2	F	0.10	0/953	0.32	0/1280
All	All	0.14	0/33348	0.38	1/44901 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	956	PRO	CA-N-CD	-9.77	98.32	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7655	0	7487	271	0
1	B	7706	0	7544	254	0
1	D	7705	0	7542	244	0
1	E	7677	0	7525	219	0
2	C	939	0	919	58	0
2	F	939	0	919	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	32621	0	31936	1043	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1043) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:724:LYS:HB2	1:E:760:ARG:HB3	1.57	0.87
1:A:98:MET:HE2	1:A:98:MET:H	1.41	0.85
1:A:309:ILE:HD11	1:A:377:GLN:HG3	1.58	0.85
1:E:395:CYS:SG	1:E:396:MET:N	2.52	0.81
1:D:247:ARG:HD2	1:D:268:ILE:HD11	1.66	0.78
1:D:250:PRO:HA	1:D:285:ARG:HH22	1.48	0.78
2:C:64:LYS:HA	2:C:217:GLU:HG3	1.66	0.78
2:C:25:ALA:HB1	2:C:63:VAL:HG21	1.67	0.77
1:D:691:ILE:HD11	1:D:716:ALA:HA	1.66	0.77
1:D:30:ILE:HD11	1:D:293:LEU:HA	1.68	0.76
1:B:124:MET:HE1	1:B:293:LEU:HB3	1.68	0.76
1:B:971:ALA:HA	1:B:1005:ILE:HD13	1.66	0.76
2:C:72:TRP:O	2:C:76:THR:OG1	2.03	0.76
1:D:447:ARG:HH12	1:D:449:GLU:HB3	1.51	0.75
1:A:1001:MET:SD	1:A:1002:ASN:ND2	2.61	0.73
1:B:759:GLU:HG2	2:C:42:ARG:HH21	1.53	0.73
1:E:973:ASN:OD1	1:E:975:HIS:ND1	2.21	0.73
1:A:214:VAL:HG22	1:A:244:PHE:HB2	1.69	0.73
1:D:60:TRP:HA	1:D:63:VAL:HG12	1.71	0.72
1:A:420:VAL:HA	1:A:423:LYS:HG2	1.71	0.72
1:D:476:ILE:HD12	1:D:477:ASN:H	1.54	0.72
1:A:724:LYS:HB2	1:A:760:ARG:HB3	1.71	0.72
1:A:831:LYS:HG3	1:A:834:GLN:HG2	1.71	0.72
1:B:804:TYR:O	1:B:808:ILE:HD12	1.87	0.72
1:A:588:LEU:HD21	1:A:612:ILE:HD13	1.71	0.71
1:E:616:MET:HE2	1:E:616:MET:HA	1.71	0.71
1:B:967:LEU:HD13	1:B:970:ILE:HD11	1.73	0.71
1:D:326:ARG:HD2	1:D:591:ASN:HD22	1.54	0.71
1:D:519:MET:HE3	1:D:522:PHE:HB3	1.71	0.71
1:D:627:ARG:NH2	1:D:672:SER:OG	2.24	0.71
1:B:227:MET:HA	1:B:227:MET:HE3	1.71	0.70
1:A:442:LEU:HD21	1:A:450:GLU:HB2	1.73	0.70
1:A:984:LEU:HD21	1:A:1000:LEU:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:ASP:OD1	1:E:380:ARG:NH1	2.25	0.70
1:E:94:VAL:HG23	1:E:95:LYS:HG2	1.74	0.69
1:A:47:GLY:O	1:A:133:ASN:ND2	2.25	0.69
1:A:568:GLU:OE1	1:A:622:LYS:NZ	2.22	0.69
1:B:620:ILE:HG21	1:B:667:LEU:HD21	1.75	0.69
1:A:364:LYS:O	1:A:370:ARG:NH2	2.26	0.69
1:A:780:VAL:HG11	1:A:819:ARG:HB3	1.75	0.69
1:B:425:ILE:HA	1:B:438:LYS:HD2	1.75	0.69
1:B:721:TYR:O	1:B:760:ARG:NH1	2.25	0.68
1:B:749:LEU:HA	1:B:753:LYS:HE2	1.75	0.68
1:D:80:SER:OG	1:D:82:ASP:OD1	2.09	0.68
1:D:668:GLU:OE2	1:D:760:ARG:NH1	2.26	0.68
1:D:831:LYS:HB2	1:D:834:GLN:HG2	1.76	0.68
1:D:622:LYS:HE2	1:D:626:GLU:HG3	1.76	0.68
1:E:342:VAL:HB	1:E:586:LEU:HD12	1.76	0.68
1:A:359:ARG:NH2	1:A:369:GLU:OE1	2.27	0.67
1:A:732:GLY:O	1:A:736:ILE:HG12	1.94	0.67
1:B:28:GLU:OE1	1:B:28:GLU:N	2.27	0.67
1:B:117:ILE:O	1:B:121:ILE:HG12	1.95	0.67
1:B:396:MET:SD	1:B:397:ALA:N	2.66	0.67
1:B:921:PHE:HB2	1:B:943:PHE:HB3	1.76	0.67
1:D:946:PRO:HB3	1:D:976:MET:HB3	1.76	0.67
1:E:119:ASP:OD1	1:E:119:ASP:N	2.28	0.67
1:B:153:SER:OG	1:B:175:ARG:NH1	2.28	0.67
1:B:342:VAL:HG11	1:B:587:ARG:HG2	1.76	0.67
1:B:973:ASN:OD1	1:B:975:HIS:ND1	2.28	0.67
1:E:519:MET:SD	1:E:519:MET:N	2.67	0.67
1:B:666:ASN:OD1	1:B:669:ARG:NH2	2.29	0.66
1:A:912:TYR:O	1:A:915:THR:OG1	2.13	0.66
1:D:539:TYR:HB3	1:D:542:LEU:HD13	1.77	0.66
1:E:768:PRO:HG2	1:E:771:ILE:HD13	1.78	0.66
1:D:930:MET:O	1:D:940:TYR:OH	2.14	0.66
1:E:327:LYS:HA	1:E:330:LEU:HD23	1.78	0.66
1:B:684:ILE:O	1:B:688:LEU:HD12	1.96	0.66
2:F:27:ALA:HA	2:F:63:VAL:HG12	1.77	0.66
1:D:647:MET:HB3	1:D:678:PHE:HA	1.77	0.65
1:E:606:HIS:HB2	2:F:205:GLU:HG3	1.78	0.65
1:D:863:ASN:O	1:D:867:ASN:ND2	2.30	0.65
1:B:688:LEU:HA	1:B:691:ILE:HG22	1.77	0.65
1:D:591:ASN:OD1	1:D:611:TYR:OH	2.14	0.65
1:A:201:SER:O	1:A:205:LYS:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ASN:O	1:B:160:ASN:ND2	2.28	0.65
1:D:324:TYR:OH	1:D:590:ASP:OD1	2.14	0.65
1:E:721:TYR:O	1:E:760:ARG:NH1	2.30	0.65
1:B:777:ASP:O	1:B:781:LEU:HD22	1.96	0.64
1:A:338:TYR:CE2	1:A:357:MET:HB2	2.33	0.64
1:D:839:PHE:HA	1:D:853:LEU:HD21	1.78	0.64
1:E:325:ILE:HD11	1:E:329:ASP:HB2	1.80	0.64
1:A:802:ARG:H	1:A:802:ARG:HD3	1.63	0.64
1:B:744:PHE:HD2	1:B:754:ARG:HH21	1.45	0.64
1:E:508:THR:HG23	1:E:511:PHE:H	1.63	0.64
1:A:551:LEU:O	1:A:555:THR:OG1	2.14	0.64
1:A:799:LEU:HD23	1:A:802:ARG:HH22	1.62	0.64
1:E:537:LYS:HA	1:E:540:LYS:HE2	1.80	0.64
1:D:684:ILE:HG21	1:D:726:VAL:HG21	1.80	0.64
1:D:775:ILE:HG21	1:D:808:ILE:HD11	1.79	0.64
1:B:348:ARG:NH2	1:B:351:ASN:O	2.31	0.63
1:D:737:VAL:HG22	1:D:758:LEU:HD11	1.80	0.63
1:A:755:TYR:CZ	1:A:807:LEU:HD23	2.33	0.63
1:B:939:GLN:HG2	1:B:943:PHE:HE1	1.64	0.63
1:A:515:ILE:HD12	1:A:516:GLU:N	2.13	0.63
1:E:320:PHE:HZ	1:E:384:LEU:HD12	1.63	0.63
1:B:791:TYR:O	1:B:833:LYS:NZ	2.28	0.63
1:A:181:GLU:OE2	1:A:182:ASN:ND2	2.32	0.63
1:A:750:ASP:HB2	1:A:753:LYS:HG2	1.81	0.63
1:B:313:TYR:O	1:B:317:SER:OG	2.14	0.62
1:B:364:LYS:NZ	1:B:394:ILE:O	2.30	0.62
1:B:838:LEU:HD12	1:B:845:LEU:HD11	1.79	0.62
1:D:115:ASN:OD1	1:D:118:HIS:ND1	2.31	0.62
1:D:962:TYR:HB3	1:D:966:LEU:HD21	1.81	0.62
1:D:237:LYS:HE3	1:D:238:ASP:HB3	1.82	0.62
1:E:98:MET:HE3	1:E:98:MET:HA	1.81	0.62
1:E:105:LYS:HA	1:E:178:PHE:HD2	1.65	0.62
1:A:163:SER:OG	1:A:164:SER:N	2.31	0.62
1:B:282:TYR:HD1	1:B:285:ARG:HH12	1.45	0.62
1:A:310:ASP:OD1	1:A:380:ARG:NH1	2.32	0.61
1:A:367:CYS:HA	1:A:370:ARG:HG2	1.82	0.61
1:A:436:TYR:OH	1:A:477:ASN:ND2	2.33	0.61
1:B:422:LYS:HA	1:B:425:ILE:HD12	1.82	0.61
1:E:554:ASP:OD2	1:E:591:ASN:ND2	2.33	0.61
1:D:509:ASP:O	1:D:513:ALA:N	2.33	0.61
1:D:980:VAL:HA	1:D:983:VAL:HG12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:838:LEU:HD11	1:D:845:LEU:HD21	1.82	0.61
1:A:227:MET:HE3	1:A:227:MET:HA	1.83	0.61
1:B:744:PHE:CE2	1:B:749:LEU:HB2	2.36	0.61
1:A:838:LEU:HD11	1:A:845:LEU:HD21	1.83	0.61
1:E:151:VAL:HG22	1:E:167:LEU:HD22	1.83	0.61
1:B:691:ILE:HD11	1:B:716:ALA:HA	1.83	0.61
1:D:421:MET:HA	1:D:424:PHE:HB2	1.83	0.61
1:E:918:ILE:HD11	1:E:966:LEU:HD11	1.83	0.61
1:B:701:ALA:O	1:B:702:ASN:ND2	2.34	0.61
1:E:870:ARG:HG2	2:F:52:ILE:HD13	1.81	0.61
1:A:304:LYS:HG2	1:A:307:GLU:HG3	1.82	0.61
1:A:820:LEU:O	1:A:824:THR:OG1	2.16	0.61
1:A:800:TYR:H	1:A:802:ARG:NH1	1.98	0.60
1:D:476:ILE:HD12	1:D:477:ASN:N	2.16	0.60
1:E:80:SER:N	1:E:83:GLU:OE1	2.34	0.60
1:E:361:PHE:HA	1:E:364:LYS:HB3	1.83	0.60
1:E:704:MET:HE1	1:E:706:VAL:HB	1.84	0.60
1:A:421:MET:HE3	1:A:441:PHE:HD1	1.66	0.60
1:B:800:TYR:H	1:B:802:ARG:HH12	1.48	0.60
1:D:613:ARG:NH1	1:D:658:HIS:O	2.34	0.60
1:D:947:GLU:HB3	1:D:975:HIS:HE1	1.67	0.60
1:E:829:GLN:HE21	1:E:832:GLN:HE22	1.49	0.60
1:A:439:ALA:HB2	1:A:454:LEU:HD23	1.84	0.60
1:A:338:TYR:OH	1:A:351:ASN:ND2	2.35	0.60
1:A:716:ALA:O	1:A:720:LEU:HG	2.02	0.60
1:E:254:GLU:N	1:E:254:GLU:OE2	2.34	0.60
1:E:348:ARG:NH2	1:E:351:ASN:OD1	2.33	0.60
1:B:498:LEU:HD21	2:C:23:PHE:HE2	1.67	0.59
2:C:172:GLU:HB2	2:C:196:PRO:HA	1.84	0.59
1:D:303:THR:OG1	1:D:304:LYS:N	2.27	0.59
2:F:225:ASP:HB2	2:F:228:THR:HG22	1.84	0.59
1:D:247:ARG:NH1	1:D:270:ASP:OD2	2.34	0.59
1:A:56:TYR:CZ	1:A:135:ASP:HB3	2.36	0.59
1:D:323:GLN:NE2	1:D:597:GLU:O	2.34	0.59
1:A:995:ARG:O	1:A:998:GLU:HG3	2.03	0.59
1:D:361:PHE:HD2	1:D:396:MET:HE2	1.68	0.59
1:E:921:PHE:HB2	1:E:943:PHE:HB3	1.84	0.59
1:A:998:GLU:O	1:A:1002:ASN:ND2	2.25	0.59
1:A:85:LEU:HD12	1:A:187:GLU:HA	1.85	0.59
1:A:118:HIS:O	1:A:122:LEU:HG	2.02	0.59
1:A:363:LEU:HB3	1:A:381:PHE:HE2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ASP:OD1	1:A:554:ASP:N	2.35	0.59
1:B:310:ASP:HA	1:B:380:ARG:HH21	1.67	0.59
1:E:984:LEU:HD21	1:E:999:ILE:HG22	1.84	0.59
1:E:776:ASP:OD2	1:E:819:ARG:NH2	2.36	0.59
1:A:938:ASP:HB2	1:A:958:TRP:HH2	1.68	0.58
1:B:341:GLU:OE2	1:B:345:THR:OG1	2.20	0.58
2:C:194:GLN:HE22	2:C:196:PRO:HB3	1.67	0.58
2:F:172:GLU:HG3	2:F:196:PRO:HA	1.85	0.58
1:A:976:MET:SD	1:A:976:MET:N	2.76	0.58
1:B:579:SER:OG	1:B:581:ASP:OD1	2.21	0.58
1:B:744:PHE:HZ	1:B:748:ASP:HB2	1.69	0.58
1:B:771:ILE:HA	1:B:774:ILE:HG12	1.85	0.58
1:D:578:MET:HE2	1:D:578:MET:HA	1.84	0.58
1:E:69:GLU:HG2	1:E:91:PHE:HE2	1.68	0.58
1:E:228:LEU:O	1:E:232:VAL:HG13	2.03	0.58
1:A:533:PHE:HA	1:A:536:GLN:HG2	1.85	0.58
1:A:707:VAL:O	1:A:710:THR:OG1	2.19	0.58
1:A:996:TYR:HA	1:A:999:ILE:HD12	1.86	0.58
2:C:14:LYS:HA	2:C:22:VAL:HG23	1.85	0.58
1:B:452:TYR:OH	1:B:518:GLU:OE1	2.21	0.58
1:D:780:VAL:HG11	1:D:819:ARG:HB3	1.84	0.58
1:B:930:MET:HE1	1:B:944:VAL:HG11	1.84	0.58
1:D:367:CYS:HA	1:D:370:ARG:HG2	1.85	0.58
1:A:313:TYR:HA	1:A:384:LEU:HD11	1.84	0.58
1:D:47:GLY:O	1:D:133:ASN:ND2	2.36	0.58
1:D:749:LEU:HD21	1:D:754:ARG:HG3	1.86	0.58
1:E:338:TYR:HA	1:E:348:ARG:HA	1.85	0.58
1:E:606:HIS:N	2:F:206:MET:O	2.37	0.58
1:D:92:TYR:HE1	1:D:97:GLU:HG2	1.69	0.58
1:D:543:GLU:OE1	1:D:543:GLU:N	2.37	0.58
1:D:827:LEU:HD13	1:D:835:ILE:HG12	1.86	0.58
1:E:534:GLU:OE1	1:E:538:LYS:NZ	2.36	0.58
1:A:936:MET:N	1:A:936:MET:HE2	2.18	0.57
1:E:579:SER:OG	1:E:581:ASP:OD1	2.21	0.57
1:B:120:LYS:HD2	1:B:290:MET:HB3	1.84	0.57
1:B:839:PHE:HA	1:B:853:LEU:HD21	1.85	0.57
1:B:854:LEU:HA	1:B:857:LYS:HB2	1.86	0.57
1:D:919:TRP:HB3	1:D:924:GLU:HB2	1.87	0.57
1:D:44:PHE:CG	1:D:121:ILE:HD11	2.40	0.57
1:A:724:LYS:HD2	1:A:760:ARG:HG2	1.86	0.57
1:A:863:ASN:O	1:A:867:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:ARG:HH22	1:B:645:PHE:HB3	1.69	0.57
2:C:26:GLU:OE1	2:C:64:LYS:NZ	2.37	0.57
1:D:967:LEU:HD21	1:D:999:ILE:HG23	1.87	0.57
1:A:776:ASP:OD2	1:A:819:ARG:NH2	2.37	0.57
1:E:253:ILE:HD12	1:E:258:LEU:HB2	1.85	0.57
1:A:827:LEU:HD11	1:A:838:LEU:HD23	1.86	0.57
1:E:348:ARG:NH2	1:E:351:ASN:O	2.36	0.57
1:A:170:VAL:HG11	1:A:204:MET:HE2	1.87	0.57
1:B:151:VAL:HG12	1:B:167:LEU:HD23	1.87	0.57
1:D:588:LEU:HD11	1:D:612:ILE:HD13	1.86	0.57
1:E:132:THR:HB	1:E:171:HIS:HD2	1.69	0.57
1:E:735:LYS:HZ1	1:E:739:ALA:HB2	1.69	0.57
1:A:748:ASP:OD1	1:A:748:ASP:N	2.29	0.56
1:E:780:VAL:HG22	1:E:820:LEU:HG	1.87	0.56
1:B:613:ARG:NE	1:B:663:ASP:OD2	2.36	0.56
1:B:926:ASN:OD1	1:B:926:ASN:N	2.37	0.56
1:E:791:TYR:O	1:E:833:LYS:NZ	2.37	0.56
1:A:613:ARG:NH1	1:A:658:HIS:O	2.38	0.56
2:C:208:LEU:HD12	2:C:208:LEU:H	1.71	0.56
1:D:724:LYS:HB2	1:D:760:ARG:HB3	1.87	0.56
1:D:46:VAL:HA	1:D:216:ILE:HG22	1.86	0.56
1:E:348:ARG:NH1	1:E:358:GLU:OE2	2.38	0.56
1:D:310:ASP:OD1	1:D:380:ARG:NH1	2.38	0.56
1:D:957:SER:HA	1:D:960:LYS:HE3	1.87	0.56
1:A:429:SER:HB2	1:A:435:ASP:OD1	2.04	0.56
1:B:121:ILE:HD13	1:B:290:MET:HE2	1.86	0.56
1:B:892:ARG:HD2	1:B:913:MET:SD	2.45	0.56
1:B:699:PHE:HD1	1:B:699:PHE:O	1.88	0.56
1:A:770:SER:O	1:A:774:ILE:HD12	2.05	0.56
1:B:205:LYS:HD3	1:B:231:TRP:CE2	2.41	0.56
2:C:219:LYS:N	2:C:219:LYS:HE2	2.21	0.56
1:A:863:ASN:ND2	1:A:866:MET:SD	2.78	0.56
1:B:554:ASP:OD1	1:B:587:ARG:NH2	2.39	0.55
1:B:804:TYR:O	1:B:807:LEU:HG	2.06	0.55
2:C:20:LYS:NZ	2:C:69:ASP:OD2	2.39	0.55
1:D:616:MET:HE2	1:D:616:MET:HA	1.87	0.55
1:A:24:ASN:O	1:A:28:GLU:HG2	2.07	0.55
1:D:785:LYS:HZ2	1:D:793:GLU:HG3	1.70	0.55
1:E:448:TRP:HB2	1:E:507:PHE:HZ	1.71	0.55
1:A:290:MET:HE3	1:A:290:MET:HA	1.88	0.55
1:E:329:ASP:HB3	1:E:541:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:O	1:A:32:GLU:HG2	2.06	0.55
1:A:771:ILE:HA	1:A:774:ILE:HD12	1.89	0.55
1:B:842:LEU:HA	1:B:845:LEU:HD13	1.89	0.55
1:A:446:GLY:HA3	1:A:708:PHE:HB2	1.88	0.55
1:B:604:SER:O	1:B:604:SER:OG	2.20	0.55
2:C:228:THR:HG22	2:C:230:GLU:HG3	1.88	0.55
1:D:540:LYS:HA	1:D:540:LYS:HE2	1.88	0.54
2:C:77:GLN:H	2:C:77:GLN:CD	2.15	0.54
1:D:436:TYR:OH	1:D:477:ASN:ND2	2.40	0.54
1:D:772:ILE:HG23	1:D:808:ILE:HD12	1.88	0.54
1:E:802:ARG:HB3	1:E:840:LYS:HB3	1.88	0.54
1:A:282:TYR:HA	1:A:285:ARG:HD2	1.89	0.54
1:A:767:LEU:HB2	1:A:771:ILE:HB	1.89	0.54
1:A:997:LEU:O	1:A:1001:MET:HG3	2.06	0.54
1:A:432:ILE:HA	1:A:435:ASP:OD2	2.08	0.54
1:A:778:PHE:HE2	1:A:804:TYR:HE2	1.56	0.54
1:A:23:ASP:OD1	1:A:24:ASN:N	2.40	0.54
1:A:421:MET:HE3	1:A:441:PHE:CD1	2.42	0.54
1:A:568:GLU:HA	1:A:571:GLU:HG2	1.90	0.54
1:D:418:TYR:HA	1:D:421:MET:HE1	1.89	0.54
1:E:59:TRP:HZ3	1:E:62:LEU:HD23	1.71	0.54
1:A:398:LYS:HE3	1:A:399:ASP:HB2	1.89	0.54
1:B:744:PHE:HZ	1:B:749:LEU:H	1.56	0.54
1:B:428:GLN:NE2	1:B:429:SER:O	2.40	0.54
1:B:648:GLU:HG3	1:B:650:TYR:H	1.72	0.54
1:B:704:MET:N	1:B:704:MET:HE3	2.23	0.54
1:B:880:GLU:O	1:B:883:GLU:HG3	2.08	0.54
1:E:866:MET:SD	1:E:866:MET:N	2.80	0.54
1:E:881:HIS:HA	1:E:884:LEU:HD23	1.90	0.54
1:B:721:TYR:HB2	1:B:757:TRP:CZ2	2.43	0.54
2:C:16:LYS:HZ1	2:C:172:GLU:HB3	1.72	0.54
1:E:373:LEU:HD12	1:E:378:TYR:CD1	2.43	0.54
1:A:35:GLU:OE1	1:A:38:ARG:NH1	2.40	0.53
1:A:939:GLN:HB2	1:A:943:PHE:CZ	2.43	0.53
1:D:29:CYS:O	1:D:33:ILE:HG12	2.08	0.53
1:E:208:ILE:HG12	1:E:213:ILE:HG13	1.89	0.53
1:E:749:LEU:HD22	1:E:753:LYS:HB3	1.90	0.53
1:B:755:TYR:HE1	1:B:807:LEU:HD23	1.73	0.53
1:B:862:ILE:O	1:B:865:LEU:N	2.40	0.53
1:B:976:MET:SD	1:B:976:MET:N	2.81	0.53
1:D:243:PRO:HG2	1:D:266:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:551:LEU:O	1:E:555:THR:OG1	2.23	0.53
1:E:897:ILE:O	1:E:903:GLY:N	2.42	0.53
1:B:915:THR:O	1:B:918:ILE:HG13	2.08	0.53
2:F:16:LYS:NZ	2:F:197:ASN:OD1	2.41	0.53
1:A:139:ASP:HA	1:A:142:CYS:SG	2.48	0.53
1:B:53:LEU:HD23	1:B:115:ASN:HD22	1.72	0.53
1:B:727:LYS:NZ	1:B:764:CYS:O	2.35	0.53
2:C:20:LYS:NZ	2:C:72:TRP:HB2	2.22	0.53
1:A:681:GLN:O	1:A:684:ILE:HG22	2.09	0.53
1:B:489:VAL:HG21	1:B:512:LEU:HD11	1.89	0.53
1:B:1002:ASN:OD1	1:B:1003:TYR:N	2.41	0.53
1:D:476:ILE:O	1:D:480:ARG:HD2	2.09	0.53
1:B:436:TYR:CE2	1:B:599:CYS:HB2	2.44	0.53
1:B:483:GLN:O	1:B:487:GLN:HG2	2.09	0.53
1:B:889:LEU:O	1:B:892:ARG:HG3	2.09	0.53
1:D:414:TYR:HA	1:D:657:ARG:HH12	1.73	0.53
1:A:358:GLU:HA	1:A:396:MET:HE1	1.90	0.53
1:A:913:MET:HE1	1:A:940:TYR:HB2	1.91	0.53
1:A:668:GLU:OE2	1:A:725:TYR:OH	2.25	0.53
1:B:862:ILE:O	1:B:865:LEU:HB2	2.09	0.53
1:E:248:THR:O	1:E:285:ARG:NH1	2.42	0.53
1:A:160:ASN:ND2	1:A:160:ASN:O	2.41	0.53
1:B:933:PHE:O	1:B:936:MET:HE1	2.09	0.53
1:B:936:MET:SD	1:B:936:MET:N	2.82	0.53
1:D:130:ILE:HD12	1:D:168:LEU:HD12	1.91	0.53
1:E:976:MET:N	1:E:976:MET:HE3	2.23	0.53
1:A:802:ARG:HH11	1:A:803:ASP:H	1.57	0.52
1:B:170:VAL:HG11	1:B:204:MET:SD	2.49	0.52
1:B:583:VAL:O	1:B:587:ARG:HG3	2.09	0.52
1:B:987:ARG:HD3	1:B:991:SER:HB3	1.91	0.52
1:E:845:LEU:O	1:E:850:LYS:NZ	2.43	0.52
1:A:37:SER:HB2	1:A:42:LEU:HD22	1.90	0.52
1:A:749:LEU:HD12	1:A:753:LYS:HB2	1.90	0.52
1:E:865:LEU:HD23	1:E:866:MET:HE1	1.92	0.52
1:A:562:THR:HG23	1:A:618:LEU:HD13	1.90	0.52
1:B:783:ALA:HA	1:B:786:HIS:CE1	2.45	0.52
1:E:681:GLN:O	1:E:684:ILE:HG13	2.09	0.52
1:A:30:ILE:HG13	1:A:293:LEU:HD22	1.90	0.52
1:B:418:TYR:HA	1:B:421:MET:HE1	1.91	0.52
1:B:491:GLN:HB2	2:C:204:PHE:CE2	2.43	0.52
1:B:769:LYS:HA	1:B:772:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:PRO:O	1:D:120:LYS:HG2	2.09	0.52
1:E:82:ASP:OD1	1:E:83:GLU:N	2.42	0.52
1:D:610:GLN:HE21	1:D:614:ASN:HD21	1.58	0.52
1:E:801:SER:HA	1:E:804:TYR:HD2	1.75	0.52
1:A:945:ASP:OD1	1:A:949:PHE:N	2.42	0.52
1:B:996:TYR:O	1:B:1000:LEU:HG	2.10	0.52
1:D:51:SER:OG	1:D:135:ASP:OD2	2.27	0.52
1:E:337:ASP:HA	1:E:350:LYS:HB3	1.91	0.52
1:E:616:MET:HB3	1:E:659:PHE:CZ	2.45	0.52
1:A:805:GLY:HA3	1:A:844:LEU:HD21	1.92	0.52
1:B:306:ASP:O	1:B:377:GLN:NE2	2.43	0.52
1:B:376:LYS:HG3	1:B:377:GLN:N	2.25	0.52
1:D:811:PHE:O	1:D:812:GLU:HG3	2.10	0.52
1:E:505:LYS:NZ	1:E:507:PHE:O	2.29	0.52
1:A:580:SER:HA	1:A:583:VAL:HG12	1.91	0.52
1:A:832:GLN:O	1:A:832:GLN:NE2	2.42	0.52
1:B:878:THR:OG1	1:B:880:GLU:OE1	2.20	0.52
1:E:373:LEU:HD12	1:E:378:TYR:HD1	1.75	0.52
1:A:802:ARG:HB3	1:A:840:LYS:HB3	1.90	0.52
1:B:421:MET:HE2	1:B:445:LEU:HD11	1.92	0.52
1:D:205:LYS:HD2	1:D:231:TRP:CE2	2.45	0.51
1:E:427:GLU:O	1:E:438:LYS:NZ	2.43	0.51
1:E:973:ASN:HB3	1:E:976:MET:HE1	1.92	0.51
1:A:224:ASN:O	1:A:228:LEU:HD23	2.11	0.51
1:D:112:LYS:HG3	1:D:113:PRO:HD2	1.91	0.51
1:A:291:ASP:HA	1:A:294:ILE:HG12	1.93	0.51
1:A:800:TYR:H	1:A:802:ARG:CZ	2.22	0.51
1:D:320:PHE:HE1	1:D:387:PHE:HB2	1.76	0.51
1:E:323:GLN:NE2	1:E:597:GLU:OE1	2.44	0.51
1:E:674:ASP:OD1	1:E:674:ASP:N	2.39	0.51
1:E:722:PHE:O	1:E:722:PHE:HD1	1.93	0.51
1:A:817:SER:HB2	1:A:820:LEU:HB2	1.92	0.51
1:B:982:GLU:HA	1:B:985:LYS:HE2	1.92	0.51
2:C:34:GLN:HE21	2:C:57:LYS:HB2	1.76	0.51
2:C:68:PHE:HD2	2:C:73:LEU:HD23	1.75	0.51
1:E:816:ILE:HD12	1:E:846:SER:HA	1.93	0.51
1:A:23:ASP:HB3	1:A:26:VAL:HG22	1.93	0.51
1:A:135:ASP:O	1:A:169:LYS:NZ	2.28	0.51
1:A:839:PHE:HA	1:A:853:LEU:HD21	1.93	0.51
1:A:889:LEU:O	1:A:893:LYS:HG2	2.10	0.51
1:B:881:HIS:O	1:B:885:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ILE:HG13	1:A:717:LYS:HD3	1.92	0.51
1:A:731:GLU:O	1:A:735:LYS:HG2	2.11	0.51
1:E:147:LYS:H	1:E:147:LYS:HD2	1.76	0.51
1:E:913:MET:HE2	1:E:913:MET:N	2.25	0.51
1:A:721:TYR:HB2	1:A:757:TRP:CE2	2.46	0.51
1:B:495:LEU:HD11	2:C:218:ILE:HD13	1.92	0.51
1:D:92:TYR:CE1	1:D:97:GLU:HG2	2.45	0.51
1:A:917:GLY:HA3	1:A:943:PHE:HD2	1.76	0.51
1:B:863:ASN:HA	1:B:866:MET:SD	2.51	0.51
1:B:984:LEU:HG	1:B:1000:LEU:HB3	1.92	0.51
2:C:204:PHE:HD1	2:C:205:GLU:N	2.09	0.51
1:E:467:ASN:OD1	1:E:468:GLY:N	2.44	0.51
1:E:962:TYR:HB3	1:E:966:LEU:HB3	1.93	0.51
1:B:786:HIS:CD2	1:B:834:GLN:HG2	2.46	0.50
1:D:90:ILE:O	1:D:94:VAL:HG12	2.11	0.50
1:E:479:TYR:HD2	1:E:524:ILE:HD12	1.76	0.50
1:E:827:LEU:HD22	1:E:838:LEU:HD12	1.93	0.50
1:A:960:LYS:HZ1	1:A:995:ARG:HB3	1.75	0.50
1:D:304:LYS:HG2	1:D:307:GLU:HG3	1.92	0.50
1:E:54:SER:HB2	1:E:115:ASN:OD1	2.11	0.50
1:E:768:PRO:HD2	1:E:771:ILE:HB	1.93	0.50
1:B:751:ILE:HD11	1:B:804:TYR:HE2	1.76	0.50
1:B:750:ASP:OD2	1:B:796:SER:N	2.43	0.50
1:B:758:LEU:O	1:B:761:LEU:HD12	2.12	0.50
1:E:62:LEU:HD13	1:E:107:PHE:CG	2.46	0.50
1:E:419:ASP:OD1	1:E:419:ASP:N	2.45	0.50
1:A:205:LYS:HE2	1:A:231:TRP:CE2	2.46	0.50
1:A:309:ILE:HD11	1:A:377:GLN:CG	2.37	0.50
1:A:624:GLU:HG2	1:A:671:CYS:HB3	1.93	0.50
1:D:447:ARG:HG2	1:D:705:ASN:HD21	1.75	0.50
1:B:214:VAL:HG22	1:B:244:PHE:HB2	1.92	0.50
1:E:60:TRP:CE2	1:E:61:ARG:HD2	2.46	0.50
1:A:206:THR:HG21	1:B:206:THR:HG21	1.93	0.50
1:A:666:ASN:OD1	1:A:669:ARG:NH2	2.43	0.50
1:A:864:ASP:HA	1:A:867:ASN:HD21	1.76	0.50
1:D:827:LEU:HD11	1:D:838:LEU:HD23	1.93	0.50
1:D:974:LYS:HA	1:D:977:LYS:HD3	1.92	0.50
1:E:210:THR:HG23	1:E:211:HIS:ND1	2.27	0.50
1:E:433:GLU:OE1	1:E:433:GLU:N	2.43	0.50
2:F:231:MET:SD	2:F:231:MET:N	2.85	0.50
1:B:375:LYS:HA	1:B:378:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:PHE:CZ	1:B:748:ASP:HB2	2.47	0.50
1:B:744:PHE:HE2	1:B:749:LEU:HB2	1.77	0.50
1:D:305:ASP:O	1:D:309:ILE:HG22	2.11	0.50
1:D:930:MET:HE3	1:D:940:TYR:CE1	2.47	0.50
1:A:720:LEU:HB2	1:A:757:TRP:CD1	2.47	0.49
1:A:759:GLU:O	1:A:763:LYS:HG2	2.12	0.49
1:D:82:ASP:OD1	1:D:83:GLU:N	2.45	0.49
1:A:318:PRO:O	1:A:539:TYR:OH	2.27	0.49
1:A:728:LEU:HD12	1:A:729:SER:N	2.27	0.49
1:B:996:TYR:HA	1:B:999:ILE:HG22	1.94	0.49
1:D:123:ALA:HA	1:D:145:ARG:HH12	1.76	0.49
1:D:522:PHE:HD1	1:D:523:ASN:N	2.09	0.49
1:D:567:SER:O	1:D:571:GLU:HG2	2.12	0.49
1:D:824:THR:HB	1:D:849:ALA:HB1	1.93	0.49
2:F:173:VAL:HG12	2:F:198:VAL:HG11	1.94	0.49
1:B:655:ILE:HA	1:B:659:PHE:CD1	2.47	0.49
1:B:661:ILE:HD11	1:B:717:LYS:HG2	1.94	0.49
2:C:172:GLU:OE1	2:C:194:GLN:NE2	2.44	0.49
1:D:552:TYR:OH	1:E:557:LYS:NZ	2.31	0.49
1:A:521:ASN:N	1:A:521:ASN:OD1	2.44	0.49
1:B:866:MET:HB2	2:C:52:ILE:HD11	1.94	0.49
2:C:8:THR:O	2:C:8:THR:OG1	2.28	0.49
1:A:569:MET:HE1	1:A:625:TYR:CD1	2.47	0.49
1:B:24:ASN:O	1:B:27:VAL:N	2.45	0.49
1:B:878:THR:HG23	1:B:881:HIS:HE1	1.78	0.49
1:D:770:SER:O	1:D:773:SER:OG	2.30	0.49
1:A:709:TYR:CE1	1:A:713:ILE:HB	2.47	0.49
1:D:769:LYS:HA	1:D:772:ILE:HD12	1.93	0.49
1:D:922:LEU:HD21	1:D:966:LEU:HB2	1.93	0.49
1:A:122:LEU:HD22	1:A:142:CYS:HA	1.94	0.49
1:A:767:LEU:HD21	1:A:811:PHE:CZ	2.48	0.49
1:D:850:LYS:HD2	1:D:854:LEU:HD23	1.94	0.49
1:D:947:GLU:HB3	1:D:975:HIS:CE1	2.48	0.49
1:E:359:ARG:HH12	1:E:363:LEU:HD12	1.78	0.49
1:E:735:LYS:O	1:E:735:LYS:NZ	2.32	0.49
1:A:152:ILE:HG22	1:A:157:ASP:HB3	1.94	0.49
1:A:893:LYS:HE2	1:A:933:PHE:CD1	2.47	0.49
2:C:13:PHE:HE1	2:C:198:VAL:HG21	1.77	0.49
1:E:449:GLU:HB2	1:E:511:PHE:HE2	1.77	0.49
1:E:554:ASP:OD1	1:E:554:ASP:N	2.41	0.49
1:A:705:ASN:HD21	1:A:708:PHE:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:MET:HG3	1:B:399:ASP:H	1.77	0.49
1:D:35:GLU:OE1	1:D:38:ARG:NH1	2.45	0.49
1:D:312:ILE:HB	1:D:316:ILE:HD12	1.95	0.49
1:D:359:ARG:O	1:D:363:LEU:HG	2.12	0.49
1:D:388:PHE:HD2	1:D:393:VAL:HG21	1.77	0.49
1:E:339:HIS:N	1:E:347:VAL:O	2.45	0.49
2:F:13:PHE:O	2:F:22:VAL:N	2.44	0.49
1:A:998:GLU:HA	1:A:1001:MET:HE3	1.94	0.49
1:B:442:LEU:HD21	1:B:450:GLU:HG3	1.95	0.49
1:D:661:ILE:HD11	1:D:717:LYS:HB3	1.94	0.49
1:E:551:LEU:HD22	1:E:608:PHE:HB2	1.94	0.49
1:A:960:LYS:NZ	1:A:995:ARG:HB3	2.28	0.48
1:A:975:HIS:HB2	1:A:976:MET:SD	2.53	0.48
1:D:448:TRP:HB2	1:D:485:ILE:HD11	1.95	0.48
1:D:776:ASP:OD1	1:D:819:ARG:NH2	2.45	0.48
1:D:820:LEU:O	1:D:824:THR:OG1	2.28	0.48
1:E:862:ILE:HD11	1:E:888:TYR:HB2	1.93	0.48
1:A:769:LYS:HA	1:A:772:ILE:HD12	1.94	0.48
1:B:742:PHE:HE1	1:B:774:ILE:HG22	1.78	0.48
1:A:799:LEU:HA	1:A:802:ARG:HH22	1.78	0.48
1:B:554:ASP:HA	1:B:587:ARG:HH22	1.78	0.48
1:D:27:VAL:O	1:D:30:ILE:HG22	2.12	0.48
1:D:99:ALA:O	1:D:103:ILE:HG22	2.14	0.48
1:E:206:THR:O	1:E:210:THR:HG22	2.12	0.48
1:E:654:ASN:OD1	1:E:654:ASN:N	2.41	0.48
1:E:655:ILE:HG21	1:E:722:PHE:HE2	1.78	0.48
1:A:83:GLU:OE1	1:A:83:GLU:N	2.46	0.48
1:A:309:ILE:C	1:A:309:ILE:HD12	2.39	0.48
1:B:808:ILE:HG23	1:B:812:GLU:OE2	2.13	0.48
1:D:229:LEU:HD13	1:D:264:LYS:HG2	1.94	0.48
1:E:360:PHE:HE1	1:E:381:PHE:HD1	1.61	0.48
1:A:884:LEU:O	1:A:887:GLU:HG3	2.13	0.48
1:B:808:ILE:O	1:B:812:GLU:HB2	2.12	0.48
1:A:312:ILE:HD12	1:A:384:LEU:HD12	1.95	0.48
1:A:767:LEU:HD23	1:A:767:LEU:H	1.78	0.48
1:B:230:ASN:HA	1:B:233:ARG:HD3	1.94	0.48
1:D:31:LYS:HA	1:D:34:THR:HG22	1.95	0.48
1:D:361:PHE:CD2	1:D:396:MET:HE2	2.48	0.48
1:D:693:GLU:O	1:D:696:THR:OG1	2.27	0.48
1:E:714:SER:HA	1:E:717:LYS:HE3	1.96	0.48
1:B:980:VAL:O	1:B:984:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:77:GLN:OE1	2:C:77:GLN:N	2.31	0.48
1:E:42:LEU:O	1:E:127:ALA:N	2.39	0.48
1:E:539:TYR:HB3	1:E:542:LEU:HD13	1.96	0.48
1:A:418:TYR:O	1:A:421:MET:HB2	2.14	0.48
1:B:771:ILE:HD12	1:B:772:ILE:N	2.28	0.48
1:D:531:MET:HE3	1:D:532:PRO:HD2	1.96	0.48
1:E:179:LYS:HG3	1:E:181:GLU:HG2	1.95	0.48
1:E:661:ILE:HD12	1:E:662:ASP:N	2.28	0.48
1:A:290:MET:O	1:A:294:ILE:HG23	2.13	0.48
1:A:731:GLU:H	1:A:731:GLU:CD	2.22	0.48
1:B:456:SER:OG	1:B:478:ARG:NH1	2.46	0.48
1:B:970:ILE:HD13	1:B:1005:ILE:HG12	1.96	0.48
1:E:805:GLY:HA2	1:E:808:ILE:HD12	1.95	0.48
1:A:807:LEU:HA	1:A:810:HIS:ND1	2.28	0.48
1:D:980:VAL:O	1:D:984:LEU:N	2.40	0.48
1:E:395:CYS:SG	1:E:399:ASP:HB3	2.54	0.48
1:A:652:PHE:CD2	1:A:684:ILE:HD11	2.49	0.47
1:A:652:PHE:CD2	1:A:722:PHE:HE1	2.32	0.47
1:B:436:TYR:HE2	1:B:599:CYS:HB2	1.79	0.47
1:B:893:LYS:NZ	1:B:932:GLU:O	2.45	0.47
1:D:220:LEU:HD13	1:D:245:PHE:CE2	2.49	0.47
1:E:59:TRP:CZ3	1:E:62:LEU:HD23	2.49	0.47
1:A:222:ASP:OD1	1:A:225:ILE:HG12	2.14	0.47
1:A:250:PRO:HA	1:A:285:ARG:CZ	2.44	0.47
1:A:934:ILE:HG12	1:A:944:VAL:HG11	1.96	0.47
1:D:532:PRO:HG3	1:E:148:TYR:CE2	2.49	0.47
1:A:24:ASN:O	1:A:27:VAL:HG12	2.15	0.47
1:A:662:ASP:OD1	1:A:663:ASP:N	2.46	0.47
1:A:721:TYR:HB2	1:A:757:TRP:CZ2	2.49	0.47
1:B:271:ALA:HB1	1:B:285:ARG:HB3	1.96	0.47
1:B:647:MET:SD	1:B:678:PHE:HA	2.55	0.47
2:C:176:ARG:HB2	2:C:192:TYR:HB3	1.96	0.47
1:D:422:LYS:HG3	1:D:445:LEU:HD11	1.96	0.47
1:D:735:LYS:HD2	1:D:735:LYS:O	2.14	0.47
1:E:744:PHE:HE1	1:E:748:ASP:HB2	1.79	0.47
1:E:946:PRO:O	1:E:951:TYR:OH	2.27	0.47
1:A:339:HIS:HB3	1:A:347:VAL:HG12	1.95	0.47
1:A:801:SER:O	1:A:804:TYR:HB2	2.14	0.47
2:C:27:ALA:HA	2:C:63:VAL:HG23	1.95	0.47
1:D:364:LYS:O	1:D:370:ARG:NH2	2.46	0.47
1:D:324:TYR:CG	1:D:593:ARG:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:735:LYS:HD2	1:D:735:LYS:C	2.39	0.47
1:A:27:VAL:O	1:A:31:LYS:HG2	2.14	0.47
1:B:366:SER:OG	1:B:367:CYS:N	2.47	0.47
1:B:724:LYS:HB2	1:B:760:ARG:HB3	1.96	0.47
1:B:918:ILE:HG22	1:B:943:PHE:CE2	2.49	0.47
1:A:984:LEU:HD12	1:A:996:TYR:HB3	1.97	0.47
1:B:561:LEU:HD13	1:B:580:SER:HB3	1.96	0.47
1:B:768:PRO:O	1:B:772:ILE:HG13	2.15	0.47
1:D:250:PRO:HA	1:D:285:ARG:NH2	2.24	0.47
1:D:255:ASN:O	1:D:259:ILE:HG13	2.15	0.47
1:D:508:THR:HG23	1:D:511:PHE:H	1.79	0.47
1:D:888:TYR:HD2	1:D:916:PHE:HZ	1.62	0.47
1:E:425:ILE:HA	1:E:438:LYS:HE2	1.96	0.47
1:E:448:TRP:N	1:E:448:TRP:CD1	2.82	0.47
1:E:728:LEU:HD12	1:E:729:SER:H	1.79	0.47
1:A:552:TYR:CE2	1:B:553:ASP:HA	2.50	0.47
1:B:229:LEU:O	1:B:233:ARG:HG3	2.14	0.47
1:D:517:ARG:O	1:D:521:ASN:ND2	2.47	0.47
1:A:124:MET:HE3	1:A:124:MET:HB3	1.69	0.47
1:A:255:ASN:OD1	1:A:256:GLU:N	2.47	0.47
2:C:28:GLN:OE1	2:C:64:LYS:HB3	2.14	0.47
1:B:201:SER:O	1:B:205:LYS:HG3	2.14	0.47
1:B:620:ILE:HD13	1:B:667:LEU:HD21	1.96	0.47
2:C:61:LEU:HB2	2:C:220:PHE:CE1	2.50	0.47
1:D:930:MET:HE3	1:D:940:TYR:CZ	2.51	0.47
1:E:205:LYS:HD2	1:E:231:TRP:CE2	2.50	0.47
1:E:482:TYR:CG	1:E:519:MET:HG3	2.50	0.47
1:A:938:ASP:HB3	1:A:953:LYS:HD3	1.96	0.46
1:B:655:ILE:O	1:B:659:PHE:HB2	2.16	0.46
1:B:737:VAL:HG11	1:B:771:ILE:HG22	1.96	0.46
1:B:966:LEU:O	1:B:970:ILE:HG13	2.14	0.46
1:B:989:LYS:HB3	1:B:989:LYS:HE2	1.74	0.46
1:D:545:LEU:H	1:D:545:LEU:HD12	1.80	0.46
1:E:245:PHE:HB2	1:E:266:LEU:HD22	1.96	0.46
1:E:337:ASP:HB3	1:E:351:ASN:HB2	1.97	0.46
1:A:27:VAL:O	1:A:30:ILE:HG22	2.15	0.46
1:B:892:ARG:NH2	1:B:936:MET:HG3	2.30	0.46
2:C:26:GLU:C	2:C:63:VAL:HG23	2.40	0.46
1:E:366:SER:OG	1:E:367:CYS:N	2.48	0.46
1:E:469:CYS:HA	1:E:535:PHE:HE2	1.80	0.46
1:E:741:LEU:HA	1:E:754:ARG:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:930:MET:HE3	1:E:930:MET:HB3	1.78	0.46
2:F:12:TYR:HB3	2:F:21:LEU:HD11	1.97	0.46
1:A:532:PRO:HG3	1:B:148:TYR:CE2	2.51	0.46
1:E:447:ARG:HB3	1:E:450:GLU:HG3	1.97	0.46
1:E:497:LEU:HD21	1:E:503:HIS:HB2	1.96	0.46
1:A:60:TRP:HA	1:A:63:VAL:HG12	1.96	0.46
1:A:662:ASP:HA	1:A:665:LYS:HD3	1.98	0.46
1:B:551:LEU:O	1:B:555:THR:HG23	2.16	0.46
1:D:291:ASP:HA	1:D:294:ILE:HG22	1.96	0.46
1:E:361:PHE:HB2	1:E:396:MET:HE1	1.98	0.46
1:D:479:TYR:HD1	1:D:519:MET:HE1	1.80	0.46
1:E:329:ASP:HA	1:E:332:HIS:ND1	2.31	0.46
1:B:179:LYS:HA	1:B:179:LYS:HD3	1.71	0.46
1:B:487:GLN:HG3	2:C:206:MET:HB2	1.97	0.46
1:B:609:HIS:O	1:B:613:ARG:HG2	2.15	0.46
2:C:48:LYS:HB3	2:C:49:PRO:HD3	1.97	0.46
2:C:218:ILE:HD12	2:C:219:LYS:H	1.80	0.46
1:D:358:GLU:HA	1:D:396:MET:HE1	1.98	0.46
1:D:655:ILE:HD12	1:D:659:PHE:CG	2.51	0.46
1:D:678:PHE:O	1:D:681:GLN:NE2	2.49	0.46
1:D:775:ILE:HD13	1:D:808:ILE:HD11	1.98	0.46
1:E:609:HIS:ND1	1:E:658:HIS:HD2	2.14	0.46
1:A:206:THR:O	1:A:210:THR:HG22	2.15	0.46
1:B:778:PHE:HA	1:B:781:LEU:HD23	1.97	0.46
2:C:27:ALA:HB3	2:C:175:TYR:CZ	2.51	0.46
1:D:237:LYS:HG3	1:D:238:ASP:OD1	2.15	0.46
1:D:247:ARG:HG2	1:D:270:ASP:HA	1.98	0.46
1:D:984:LEU:HD11	1:D:1005:ILE:HD12	1.97	0.46
1:E:214:VAL:HG22	1:E:244:PHE:HB2	1.96	0.46
2:F:193:ILE:HD12	2:F:234:VAL:HB	1.97	0.46
1:A:63:VAL:HG11	1:A:84:TYR:CE1	2.51	0.46
1:A:357:MET:HE1	1:A:360:PHE:HD2	1.81	0.46
1:A:627:ARG:HH12	1:A:676:ILE:HA	1.81	0.46
1:A:874:ILE:HD13	1:A:881:HIS:HE1	1.81	0.46
1:B:850:LYS:O	1:B:854:LEU:HG	2.16	0.46
2:C:60:ASN:OD1	2:C:61:LEU:N	2.49	0.46
1:D:828:THR:OG1	1:D:830:ASP:OD1	2.29	0.46
1:E:220:LEU:HG	1:E:245:PHE:HE2	1.81	0.46
1:E:312:ILE:HG21	1:E:360:PHE:HE2	1.81	0.46
1:E:358:GLU:OE1	1:E:358:GLU:N	2.45	0.46
1:A:549:GLN:OE1	1:A:549:GLN:N	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:TYR:HD2	1:D:480:ARG:HE	1.62	0.46
1:E:585:LEU:HD12	1:E:585:LEU:HA	1.81	0.46
1:A:733:LEU:O	1:A:737:VAL:HG13	2.16	0.46
1:E:390:LYS:HG2	1:E:391:ASN:HD22	1.80	0.46
1:A:709:TYR:HD1	1:A:709:TYR:O	1.99	0.45
1:D:105:LYS:HZ2	1:D:105:LYS:C	2.24	0.45
1:D:435:ASP:HB3	1:D:458:ILE:HD12	1.98	0.45
1:E:35:GLU:OE2	1:E:35:GLU:HA	2.15	0.45
1:E:115:ASN:HB2	1:E:118:HIS:ND1	2.30	0.45
1:E:927:ASN:HD21	1:E:929:LYS:HD3	1.81	0.45
1:A:395:CYS:SG	1:A:396:MET:N	2.88	0.45
1:A:685:GLU:HB2	1:A:728:LEU:HD13	1.97	0.45
1:A:866:MET:O	1:A:869:ILE:HG13	2.16	0.45
1:B:418:TYR:HD1	1:B:418:TYR:H	1.64	0.45
1:D:155:GLU:O	1:D:158:VAL:HG12	2.16	0.45
1:D:384:LEU:HD12	1:D:384:LEU:H	1.81	0.45
1:D:750:ASP:OD2	1:D:796:SER:OG	2.35	0.45
1:E:54:SER:O	1:E:54:SER:OG	2.31	0.45
2:F:174:GLU:HG2	2:F:194:GLN:HA	1.98	0.45
1:A:563:ASN:ND2	1:B:614:ASN:OD1	2.50	0.45
1:A:727:LYS:HD3	1:A:728:LEU:N	2.30	0.45
1:A:959:LEU:HA	1:A:962:TYR:CD2	2.52	0.45
1:B:732:GLY:O	1:B:736:ILE:HD13	2.15	0.45
1:A:45:PHE:HD2	1:A:218:TYR:HE2	1.65	0.45
2:C:72:TRP:HA	2:C:75:MET:SD	2.56	0.45
1:D:155:GLU:OE1	1:D:197:TYR:HA	2.17	0.45
1:D:398:LYS:HE3	1:D:398:LYS:HB3	1.77	0.45
1:D:974:LYS:HB3	1:D:974:LYS:HE3	1.60	0.45
1:A:771:ILE:H	1:A:771:ILE:HD12	1.81	0.45
1:B:418:TYR:HD2	1:B:708:PHE:HZ	1.63	0.45
1:B:497:LEU:HD12	1:B:497:LEU:H	1.82	0.45
1:B:513:ALA:O	1:B:516:GLU:HG3	2.17	0.45
1:D:308:VAL:HG13	1:D:356:TYR:HB2	1.98	0.45
1:D:459:ILE:HG23	1:D:471:TYR:HE1	1.82	0.45
1:D:999:ILE:HG22	1:D:1005:ILE:HD11	1.97	0.45
1:E:306:ASP:O	1:E:377:GLN:NE2	2.49	0.45
1:A:341:GLU:OE1	1:A:341:GLU:N	2.50	0.45
1:B:410:ASN:OD1	1:B:410:ASN:N	2.50	0.45
1:D:284:GLU:N	1:D:284:GLU:OE1	2.50	0.45
1:E:831:LYS:HB2	1:E:834:GLN:HB2	1.98	0.45
1:A:86:ARG:O	1:A:90:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:LEU:HD13	1:B:811:PHE:CG	2.52	0.45
2:C:13:PHE:CE1	2:C:198:VAL:HG21	2.51	0.45
1:D:480:ARG:HB2	1:D:601:TRP:HD1	1.81	0.45
1:D:920:TYR:OH	1:D:931:GLU:OE2	2.21	0.45
1:E:796:SER:HA	2:F:223:LEU:HA	1.98	0.45
1:E:842:LEU:HA	1:E:845:LEU:HD12	1.99	0.45
2:F:28:GLN:HG2	2:F:29:THR:OG1	2.17	0.45
1:A:86:ARG:HG2	1:A:90:ILE:HD11	1.99	0.45
1:A:569:MET:HE1	1:A:625:TYR:CG	2.52	0.45
1:B:29:CYS:O	1:B:33:ILE:HG22	2.17	0.45
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.84	0.45
1:B:674:ASP:HA	1:B:725:TYR:HE2	1.82	0.45
1:B:727:LYS:HD2	1:B:727:LYS:HA	1.78	0.45
1:B:770:SER:O	1:B:774:ILE:HG12	2.17	0.45
1:D:686:GLU:O	1:D:690:GLY:N	2.43	0.45
1:E:215:PHE:HB2	1:E:245:PHE:HD1	1.82	0.45
1:E:777:ASP:HB3	1:E:819:ARG:NH1	2.31	0.45
1:A:954:PHE:HD2	1:A:979:HIS:CD2	2.34	0.45
1:B:309:ILE:HD13	1:B:309:ILE:HA	1.84	0.45
1:B:869:ILE:HG12	1:B:874:ILE:HB	1.99	0.45
2:C:174:GLU:OE2	2:C:192:TYR:HB2	2.17	0.45
1:D:132:THR:HB	1:D:171:HIS:HD2	1.82	0.45
1:D:228:LEU:O	1:D:232:VAL:HG13	2.17	0.45
1:D:422:LYS:O	1:D:426:GLU:HG2	2.17	0.45
1:D:450:GLU:H	1:D:450:GLU:HG2	1.63	0.45
1:E:418:TYR:O	1:E:422:LYS:HG3	2.16	0.45
1:E:818:LYS:HB2	1:E:818:LYS:HE2	1.70	0.45
1:A:552:TYR:HE2	1:B:553:ASP:HA	1.81	0.45
1:A:819:ARG:HA	1:A:822:GLU:OE1	2.17	0.45
1:D:380:ARG:O	1:D:384:LEU:HD12	2.17	0.45
1:D:479:TYR:CD1	1:D:519:MET:HE1	2.52	0.45
1:D:674:ASP:OD1	1:D:674:ASP:N	2.50	0.45
1:D:874:ILE:HD11	1:D:878:THR:HG23	1.99	0.45
1:E:473:LEU:HD12	1:E:473:LEU:H	1.81	0.45
1:E:678:PHE:HE2	1:E:722:PHE:HE1	1.64	0.45
1:B:173:ASP:OD1	1:B:174:PHE:N	2.47	0.44
1:B:427:GLU:O	1:B:438:LYS:NZ	2.50	0.44
1:B:648:GLU:OE1	1:B:649:TYR:N	2.46	0.44
1:E:602:SER:HA	1:E:605:PHE:CD1	2.52	0.44
1:E:960:LYS:NZ	1:E:995:ARG:HG3	2.32	0.44
1:D:315:LYS:HZ3	1:D:334:PHE:HD1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:582:ILE:HD13	1:D:582:ILE:HA	1.88	0.44
1:E:423:LYS:O	1:E:427:GLU:HG3	2.17	0.44
1:E:736:ILE:HG13	1:E:737:VAL:N	2.32	0.44
1:E:742:PHE:HE2	1:E:774:ILE:HG23	1.82	0.44
2:F:8:THR:O	2:F:8:THR:OG1	2.25	0.44
1:A:709:TYR:HE1	1:A:713:ILE:HB	1.82	0.44
1:A:755:TYR:O	1:A:758:LEU:HD12	2.18	0.44
1:B:419:ASP:HA	1:B:422:LYS:NZ	2.32	0.44
1:B:752:GLY:HA3	1:B:795:SER:HB2	2.00	0.44
1:B:766:GLU:O	1:B:768:PRO:HD3	2.17	0.44
2:C:70:LEU:HD12	2:C:71:GLU:N	2.31	0.44
1:D:27:VAL:O	1:D:31:LYS:HG2	2.17	0.44
1:D:118:HIS:O	1:D:121:ILE:HG22	2.18	0.44
1:D:478:ARG:NH2	1:D:518:GLU:OE2	2.51	0.44
1:E:41:LYS:HB3	1:E:41:LYS:HE2	1.68	0.44
1:E:229:LEU:HD12	1:E:264:LYS:HB3	1.99	0.44
1:E:559:PHE:CD1	1:E:559:PHE:C	2.95	0.44
1:E:655:ILE:O	1:E:659:PHE:HB2	2.17	0.44
1:E:820:LEU:O	1:E:824:THR:OG1	2.33	0.44
1:B:186:LYS:H	1:B:186:LYS:HD3	1.82	0.44
1:B:326:ARG:HG3	1:B:594:PHE:HB2	1.98	0.44
1:B:673:ILE:O	1:B:676:ILE:HG22	2.17	0.44
1:D:316:ILE:HD13	1:D:384:LEU:HD23	1.98	0.44
1:D:885:ILE:HG23	1:D:916:PHE:CE1	2.52	0.44
1:E:247:ARG:NH2	1:E:249:ASP:HB3	2.32	0.44
1:E:477:ASN:O	1:E:481:ILE:HG12	2.18	0.44
1:A:447:ARG:HB3	1:A:450:GLU:OE2	2.17	0.44
1:A:763:LYS:HA	1:A:763:LYS:HD3	1.76	0.44
1:A:785:LYS:NZ	1:A:788:ASP:OD1	2.50	0.44
1:A:960:LYS:HA	1:A:995:ARG:NH1	2.33	0.44
1:A:997:LEU:HA	1:A:1000:LEU:HG	2.00	0.44
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.85	0.44
1:B:396:MET:SD	1:B:398:LYS:HG2	2.58	0.44
1:B:423:LYS:HA	1:B:426:GLU:HG2	2.00	0.44
1:B:985:LYS:HA	1:B:988:VAL:HG12	2.00	0.44
1:E:29:CYS:O	1:E:33:ILE:HG12	2.18	0.44
1:E:491:GLN:HB2	2:F:204:PHE:CZ	2.53	0.44
1:A:883:GLU:O	1:A:886:ILE:HG22	2.17	0.44
1:B:750:ASP:OD1	1:B:753:LYS:HG3	2.18	0.44
1:B:831:LYS:HB2	1:B:834:GLN:HG3	2.00	0.44
1:B:862:ILE:HG22	1:B:866:MET:HE1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:TYR:HE1	1:D:103:ILE:HG21	1.82	0.44
1:D:985:LYS:HB2	1:D:989:LYS:HE2	2.00	0.44
1:A:380:ARG:O	1:A:384:LEU:HG	2.17	0.44
1:A:627:ARG:NH1	1:A:676:ILE:HA	2.33	0.44
1:D:937:ASP:OD1	1:D:938:ASP:N	2.50	0.44
1:E:179:LYS:HG3	1:E:181:GLU:H	1.82	0.44
1:E:339:HIS:CE1	1:E:341:GLU:HB3	2.53	0.44
1:E:976:MET:HG2	1:E:980:VAL:HG23	1.99	0.44
1:A:734:GLY:HA2	1:A:737:VAL:HG22	2.00	0.44
1:A:965:LYS:HE3	1:A:965:LYS:HB3	1.64	0.44
2:C:11:VAL:HB	2:C:25:ALA:HB3	2.00	0.44
2:C:14:LYS:HD3	2:C:172:GLU:OE2	2.18	0.44
2:C:204:PHE:CD1	2:C:204:PHE:C	2.95	0.44
1:D:559:PHE:CD2	1:E:559:PHE:HB2	2.52	0.44
1:D:913:MET:SD	1:D:939:GLN:NE2	2.91	0.44
1:E:948:ASN:OD1	1:E:948:ASN:N	2.49	0.44
1:A:879:PRO:HA	1:A:882:GLU:CD	2.43	0.44
1:B:977:LYS:NZ	1:B:1004:PHE:O	2.51	0.44
1:D:384:LEU:HB3	1:D:388:PHE:CE1	2.53	0.44
1:E:586:LEU:HA	1:E:589:TYR:CE2	2.53	0.44
1:A:210:THR:HG23	1:A:211:HIS:ND1	2.33	0.43
1:A:937:ASP:HB3	1:A:939:GLN:NE2	2.33	0.43
1:B:364:LYS:HA	1:B:381:PHE:HZ	1.83	0.43
1:B:742:PHE:CZ	1:B:778:PHE:HB2	2.53	0.43
1:E:613:ARG:HA	1:E:659:PHE:CZ	2.53	0.43
1:A:360:PHE:O	1:A:363:LEU:HB2	2.17	0.43
1:B:958:TRP:HB3	1:B:962:TYR:OH	2.19	0.43
1:D:55:ASP:O	1:D:112:LYS:HG2	2.17	0.43
1:D:64:ASP:OD1	1:D:65:LYS:N	2.51	0.43
1:D:447:ARG:NH2	1:D:450:GLU:OE1	2.49	0.43
1:D:801:SER:O	1:D:841:LEU:HD21	2.18	0.43
1:A:817:SER:OG	1:A:844:LEU:O	2.35	0.43
1:A:920:TYR:CE1	1:A:944:VAL:HA	2.54	0.43
1:B:274:LEU:HD12	1:B:274:LEU:HA	1.82	0.43
1:B:778:PHE:CD1	1:B:778:PHE:C	2.96	0.43
1:B:949:PHE:CE2	1:B:951:TYR:HA	2.53	0.43
1:E:361:PHE:CD1	1:E:364:LYS:HD2	2.52	0.43
1:E:500:PHE:HD1	1:E:502:ARG:HG2	1.84	0.43
1:E:908:SER:OG	1:E:909:SER:N	2.51	0.43
2:F:199:SER:OG	2:F:221:GLU:OE2	2.30	0.43
2:C:11:VAL:HG22	2:C:175:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:LYS:HZ1	2:C:72:TRP:HB2	1.83	0.43
1:D:309:ILE:HA	1:D:312:ILE:HD11	2.00	0.43
1:D:513:ALA:O	1:D:517:ARG:HG2	2.19	0.43
1:A:111:ASP:OD1	1:A:111:ASP:N	2.49	0.43
1:B:364:LYS:HE3	1:B:385:PHE:HE1	1.84	0.43
1:D:246:ILE:HD13	1:D:269:ILE:HB	2.00	0.43
1:A:607:GLU:H	1:A:607:GLU:HG2	1.63	0.43
1:A:1000:LEU:HD12	1:A:1001:MET:N	2.33	0.43
1:B:144:LYS:HE3	1:B:144:LYS:HB3	1.85	0.43
1:B:724:LYS:HE3	1:B:763:LYS:HG2	2.00	0.43
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.83	0.43
1:D:338:TYR:CD1	1:D:348:ARG:HA	2.53	0.43
1:D:988:VAL:HG11	1:D:997:LEU:HD13	2.01	0.43
1:A:278:ASN:HB3	1:A:281:ASP:OD1	2.18	0.43
1:A:946:PRO:HB3	1:A:976:MET:SD	2.59	0.43
1:B:258:LEU:O	1:B:262:GLU:HG3	2.19	0.43
1:B:587:ARG:HA	1:B:590:ASP:OD2	2.19	0.43
1:B:974:LYS:O	1:B:974:LYS:NZ	2.25	0.43
1:B:1002:ASN:C	1:B:1003:TYR:HD1	2.26	0.43
2:C:40:LYS:HG3	2:C:41:LEU:HG	2.01	0.43
2:C:222:ALA:HB1	2:C:231:MET:HE2	2.00	0.43
1:D:229:LEU:HA	1:D:232:VAL:HG22	2.00	0.43
1:A:46:VAL:HB	1:A:131:THR:HB	2.00	0.43
1:B:818:LYS:HB2	1:B:818:LYS:HE2	1.65	0.43
2:C:13:PHE:HA	2:C:173:VAL:HG23	2.01	0.43
1:D:588:LEU:CD2	1:D:616:MET:HE3	2.48	0.43
1:D:647:MET:HG2	1:D:678:PHE:CE2	2.54	0.43
1:D:919:TRP:HE3	1:D:925:ILE:HD11	1.84	0.43
1:E:796:SER:HB3	2:F:223:LEU:HD23	2.00	0.43
2:F:40:LYS:HE2	2:F:40:LYS:HB2	1.79	0.43
1:A:98:MET:HE2	1:A:98:MET:N	2.22	0.43
1:A:358:GLU:HA	1:A:396:MET:CE	2.48	0.43
1:A:534:GLU:O	1:A:538:LYS:HB2	2.19	0.43
1:B:646:PHE:HB3	1:B:677:ARG:HH21	1.83	0.43
1:B:967:LEU:HB3	1:B:1003:TYR:CD2	2.54	0.43
1:D:448:TRP:HB3	1:D:481:ILE:HD11	2.00	0.43
1:E:27:VAL:O	1:E:30:ILE:HG22	2.18	0.43
1:E:345:THR:HB	1:E:397:ALA:HA	2.00	0.43
1:A:374:SER:O	1:A:378:TYR:N	2.44	0.43
1:A:553:ASP:OD1	1:A:553:ASP:C	2.62	0.43
1:B:359:ARG:HH21	1:B:363:LEU:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:LYS:HA	1:B:538:LYS:HD3	1.72	0.43
1:B:771:ILE:O	1:B:775:ILE:HG22	2.19	0.43
1:B:865:LEU:HD23	1:B:865:LEU:HA	1.78	0.43
1:B:914:SER:O	1:B:918:ILE:HG23	2.19	0.43
1:D:588:LEU:HD12	1:D:588:LEU:HA	1.90	0.43
1:E:376:LYS:HD2	1:E:377:GLN:HG2	2.01	0.43
1:A:657:ARG:HG2	1:A:658:HIS:CD2	2.54	0.42
1:A:967:LEU:HD23	1:A:1003:TYR:HD2	1.84	0.42
1:B:581:ASP:OD1	1:B:582:ILE:N	2.51	0.42
1:B:724:LYS:HD3	1:B:760:ARG:NH2	2.33	0.42
1:B:817:SER:OG	1:B:820:LEU:HB2	2.20	0.42
2:C:24:THR:OG1	2:C:67:PHE:HD2	2.02	0.42
1:D:521:ASN:HB2	1:E:145:ARG:NH2	2.35	0.42
1:D:741:LEU:HA	1:D:754:ARG:HE	1.84	0.42
1:E:152:ILE:HB	1:E:168:LEU:HD23	2.01	0.42
1:E:423:LYS:HD2	1:E:424:PHE:N	2.34	0.42
1:E:593:ARG:O	1:E:597:GLU:HB2	2.19	0.42
1:E:616:MET:HB3	1:E:659:PHE:HZ	1.83	0.42
1:E:660:LYS:HA	1:E:660:LYS:HD3	1.82	0.42
1:E:678:PHE:HE2	1:E:722:PHE:CE1	2.36	0.42
1:A:53:LEU:HB3	1:A:115:ASN:HD22	1.84	0.42
1:A:225:ILE:O	1:A:229:LEU:HD23	2.19	0.42
1:A:753:LYS:O	1:A:757:TRP:HE3	2.02	0.42
1:B:978:HIS:O	1:B:981:ILE:HG22	2.19	0.42
1:E:205:LYS:HE2	1:E:231:TRP:CG	2.54	0.42
1:E:817:SER:OG	1:E:820:LEU:HB2	2.19	0.42
2:F:174:GLU:OE2	2:F:192:TYR:HB2	2.19	0.42
1:A:325:ILE:HD11	1:A:541:ILE:HD12	2.02	0.42
1:A:338:TYR:HE1	1:A:351:ASN:HB2	1.85	0.42
1:A:421:MET:HE1	1:A:444:CYS:HB2	2.02	0.42
1:A:964:ASP:OD1	1:A:964:ASP:N	2.51	0.42
1:B:781:LEU:O	1:B:785:LYS:HG2	2.19	0.42
1:D:311:TYR:HD2	1:D:312:ILE:HG23	1.85	0.42
1:D:862:ILE:HD11	1:D:866:MET:HE3	2.01	0.42
1:E:248:THR:HA	1:E:271:ALA:HB3	2.01	0.42
1:E:984:LEU:HD12	1:E:984:LEU:HA	1.90	0.42
1:A:27:VAL:HA	1:A:30:ILE:HG22	2.01	0.42
1:A:303:THR:N	1:A:307:GLU:OE1	2.52	0.42
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.81	0.42
1:A:754:ARG:O	1:A:758:LEU:HG	2.19	0.42
1:B:304:LYS:HB2	1:B:307:GLU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:TYR:C	1:D:325:ILE:HD12	2.44	0.42
1:D:556:VAL:HG23	1:E:556:VAL:HG22	2.00	0.42
1:E:130:ILE:HG13	1:E:168:LEU:HB2	2.02	0.42
1:E:424:PHE:O	1:E:438:LYS:NZ	2.41	0.42
1:A:374:SER:HB3	1:A:377:GLN:HB2	2.02	0.42
1:A:842:LEU:HB3	1:A:843:PRO:HD3	2.02	0.42
1:B:728:LEU:HD23	1:B:728:LEU:HA	1.78	0.42
1:D:472:TYR:OH	1:D:546:SER:HB3	2.20	0.42
1:D:864:ASP:HA	1:D:867:ASN:HD21	1.84	0.42
1:D:888:TYR:HD2	1:D:916:PHE:CZ	2.37	0.42
1:E:220:LEU:HD22	1:E:261:TYR:CD2	2.55	0.42
1:E:447:ARG:HE	1:E:450:GLU:CD	2.27	0.42
1:A:788:ASP:OD1	1:A:788:ASP:N	2.52	0.42
1:B:266:LEU:HD23	1:B:266:LEU:HA	1.86	0.42
1:B:449:GLU:HB2	1:B:511:PHE:CE2	2.54	0.42
1:B:740:LEU:HD11	1:B:757:TRP:HB3	2.00	0.42
1:B:976:MET:O	1:B:980:VAL:HG23	2.20	0.42
1:D:98:MET:C	1:D:98:MET:HE3	2.45	0.42
1:D:418:TYR:HD1	1:D:421:MET:HE1	1.84	0.42
1:D:667:LEU:HB3	1:D:673:ILE:HD11	2.02	0.42
1:D:713:ILE:HD12	1:D:713:ILE:HA	1.84	0.42
1:E:277:SER:OG	1:E:278:ASN:N	2.50	0.42
1:A:613:ARG:HH11	1:A:659:PHE:HD1	1.67	0.42
1:A:728:LEU:HD12	1:A:729:SER:H	1.84	0.42
1:A:758:LEU:O	1:A:762:THR:HG23	2.20	0.42
1:B:385:PHE:O	1:B:389:GLU:HG2	2.19	0.42
1:B:593:ARG:O	1:B:597:GLU:HB2	2.20	0.42
1:B:800:TYR:N	1:B:802:ARG:HH12	2.15	0.42
2:C:16:LYS:HA	2:C:16:LYS:HD3	1.81	0.42
2:C:204:PHE:HD1	2:C:204:PHE:C	2.28	0.42
1:D:206:THR:HG21	1:E:206:THR:HG21	2.02	0.42
1:D:720:LEU:HD23	1:D:757:TRP:HD1	1.84	0.42
1:E:600:LEU:HD11	1:E:602:SER:HB2	2.02	0.42
1:A:222:ASP:OD1	1:A:222:ASP:C	2.62	0.42
1:B:290:MET:O	1:B:294:ILE:HD12	2.20	0.42
1:B:376:LYS:HA	1:B:379:GLU:OE2	2.19	0.42
1:B:588:LEU:C	1:B:588:LEU:HD23	2.45	0.42
1:B:746:GLU:OE1	1:B:746:GLU:N	2.45	0.42
1:D:311:TYR:CD2	1:D:312:ILE:HG23	2.55	0.42
1:E:479:TYR:CD2	1:E:524:ILE:HD12	2.54	0.42
1:E:500:PHE:CD1	1:E:502:ARG:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:693:GLU:O	1:E:697:LYS:HG2	2.20	0.42
1:A:308:VAL:HG13	1:A:356:TYR:HB2	2.01	0.42
1:A:977:LYS:O	1:A:981:ILE:HG12	2.20	0.42
1:D:229:LEU:HA	1:D:229:LEU:HD23	1.87	0.42
1:D:647:MET:HG2	1:D:678:PHE:CD2	2.55	0.42
1:D:660:LYS:HA	1:D:660:LYS:HD3	1.75	0.42
1:E:657:ARG:HE	1:E:715:GLU:CD	2.26	0.42
2:F:48:LYS:HB3	2:F:49:PRO:HD3	2.00	0.42
1:A:799:LEU:HD23	1:A:799:LEU:HA	1.71	0.42
1:B:558:LEU:HD11	1:B:615:SER:HA	2.02	0.42
1:B:624:GLU:HG3	1:B:671:CYS:HB2	2.01	0.42
1:B:997:LEU:HD12	1:B:998:GLU:N	2.35	0.42
2:C:172:GLU:CD	2:C:194:GLN:HE21	2.27	0.42
1:D:695:ILE:HD13	1:D:695:ILE:HA	1.93	0.42
1:E:741:LEU:HD23	1:E:754:ARG:HD3	2.02	0.42
1:A:47:GLY:HA2	1:A:218:TYR:CZ	2.55	0.41
1:B:688:LEU:HA	1:B:691:ILE:CG2	2.48	0.41
1:B:897:ILE:O	1:B:903:GLY:N	2.53	0.41
1:D:124:MET:HE3	1:D:124:MET:O	2.20	0.41
1:D:445:LEU:HD23	1:D:445:LEU:HA	1.93	0.41
1:D:512:LEU:O	1:D:515:ILE:HG22	2.20	0.41
1:D:656:SER:HB3	1:D:719:ALA:HB2	2.01	0.41
1:D:889:LEU:HD11	1:D:930:MET:HE1	2.01	0.41
1:E:448:TRP:CD1	1:E:448:TRP:H	2.38	0.41
1:B:242:LYS:HB3	1:B:242:LYS:HE2	1.87	0.41
1:B:767:LEU:HB3	1:B:771:ILE:HD11	2.01	0.41
1:B:772:ILE:HA	1:B:775:ILE:HG22	2.01	0.41
1:B:824:THR:HA	1:B:827:LEU:HB2	2.01	0.41
1:B:982:GLU:O	1:B:985:LYS:HG2	2.19	0.41
1:B:999:ILE:HA	1:B:1002:ASN:HD21	1.86	0.41
1:D:382:ASN:O	1:D:386:ASN:N	2.44	0.41
1:E:425:ILE:HG23	1:E:442:LEU:HD11	2.02	0.41
1:E:886:ILE:O	1:E:890:GLU:HG2	2.20	0.41
1:A:422:LYS:O	1:A:426:GLU:HG2	2.21	0.41
1:A:524:ILE:H	1:A:524:ILE:HG13	1.73	0.41
1:A:935:GLY:C	1:A:936:MET:HE2	2.45	0.41
1:B:326:ARG:HB2	1:B:329:ASP:OD2	2.20	0.41
1:D:290:MET:O	1:D:294:ILE:HG22	2.20	0.41
1:D:319:LEU:HD22	1:D:319:LEU:H	1.86	0.41
1:D:614:ASN:HD22	1:E:559:PHE:HZ	1.68	0.41
1:E:751:ILE:HD12	1:E:751:ILE:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:SER:N	1:A:318:PRO:HD2	2.35	0.41
1:A:807:LEU:HD12	1:A:808:ILE:N	2.35	0.41
1:B:205:LYS:HD3	1:B:231:TRP:NE1	2.36	0.41
1:B:741:LEU:HB3	1:B:778:PHE:CD2	2.55	0.41
1:B:752:GLY:HA3	1:B:797:ASN:OD1	2.20	0.41
2:C:10:ASP:OD1	2:C:10:ASP:C	2.63	0.41
2:C:11:VAL:O	2:C:24:THR:HA	2.21	0.41
1:D:662:ASP:OD1	1:D:663:ASP:N	2.53	0.41
1:D:696:THR:HA	1:D:743:TYR:CD2	2.56	0.41
1:E:932:GLU:H	1:E:932:GLU:HG2	1.73	0.41
1:A:105:LYS:HB3	1:A:105:LYS:HE2	1.88	0.41
1:B:801:SER:O	1:B:804:TYR:HB2	2.20	0.41
2:C:61:LEU:HB2	2:C:220:PHE:CD1	2.56	0.41
1:D:274:LEU:HD21	1:D:292:LEU:HD12	2.03	0.41
1:D:318:PRO:HG2	1:D:319:LEU:HD22	2.02	0.41
1:D:361:PHE:CD1	1:D:364:LYS:HE2	2.55	0.41
1:D:771:ILE:O	1:D:775:ILE:HG22	2.21	0.41
1:A:350:LYS:O	1:A:350:LYS:NZ	2.37	0.41
1:A:840:LYS:HA	1:A:871:ILE:HG12	2.01	0.41
1:B:442:LEU:HB3	1:B:451:SER:OG	2.19	0.41
1:B:865:LEU:O	1:B:869:ILE:HG13	2.20	0.41
1:B:996:TYR:O	1:B:999:ILE:HG22	2.21	0.41
1:D:547:ASP:OD1	1:D:547:ASP:N	2.49	0.41
1:A:43:VAL:HG12	1:A:128:HIS:H	1.85	0.41
1:A:580:SER:O	1:A:584:VAL:HG12	2.21	0.41
1:B:35:GLU:HA	1:B:38:ARG:HG3	2.03	0.41
1:B:186:LYS:HB2	1:B:186:LYS:HE2	1.80	0.41
1:B:206:THR:O	1:B:210:THR:HG23	2.21	0.41
1:D:613:ARG:HA	1:D:659:PHE:CE1	2.56	0.41
1:E:689:VAL:HG13	1:E:735:LYS:HG2	2.01	0.41
1:E:892:ARG:HH21	1:E:910:ASN:ND2	2.18	0.41
1:A:85:LEU:HD11	1:A:190:TYR:CD2	2.56	0.41
1:A:445:LEU:HD23	1:A:445:LEU:HA	1.92	0.41
1:A:549:GLN:HB2	1:A:552:TYR:CD1	2.55	0.41
1:A:564:LYS:O	1:A:564:LYS:HD3	2.21	0.41
1:A:695:ILE:HG12	1:A:744:PHE:CE1	2.56	0.41
1:A:737:VAL:HA	1:A:740:LEU:CD2	2.51	0.41
1:A:797:ASN:ND2	1:A:799:LEU:HB2	2.35	0.41
1:B:199:LEU:HD23	1:B:202:ASN:HD21	1.85	0.41
1:B:949:PHE:CE2	1:B:954:PHE:HD2	2.39	0.41
1:D:82:ASP:OD1	1:D:83:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:TYR:HE1	1:D:351:ASN:HB2	1.86	0.41
1:D:469:CYS:HA	1:D:535:PHE:HE2	1.84	0.41
1:D:472:TYR:O	1:D:476:ILE:HG13	2.21	0.41
1:E:60:TRP:HA	1:E:63:VAL:HG12	2.01	0.41
1:E:229:LEU:HD13	1:E:229:LEU:HA	1.88	0.41
1:E:320:PHE:CZ	1:E:384:LEU:HD12	2.50	0.41
1:E:556:VAL:HB	1:E:557:LYS:HZ2	1.85	0.41
1:E:857:LYS:HA	1:E:857:LYS:HD2	1.79	0.41
1:A:660:LYS:HA	1:A:660:LYS:HD3	1.90	0.41
1:B:424:PHE:CD1	1:B:424:PHE:C	2.99	0.41
1:B:884:LEU:HD23	1:B:884:LEU:HA	1.89	0.41
1:B:896:TYR:CD1	1:B:896:TYR:C	2.99	0.41
1:B:970:ILE:HD12	1:B:971:ALA:N	2.36	0.41
1:D:174:PHE:HD1	1:D:178:PHE:HA	1.85	0.41
1:D:331:LYS:HG2	1:D:339:HIS:HA	2.03	0.41
1:D:1005:ILE:H	1:D:1005:ILE:HG13	1.67	0.41
1:A:203:LEU:HA	1:A:206:THR:HG22	2.03	0.40
1:A:485:ILE:HD13	1:A:511:PHE:HE2	1.86	0.40
1:B:130:ILE:HD11	1:B:207:ILE:HG21	2.02	0.40
1:B:930:MET:HE2	1:B:930:MET:C	2.45	0.40
1:D:655:ILE:HA	1:D:659:PHE:CD1	2.56	0.40
1:D:844:LEU:HD12	1:D:845:LEU:HG	2.01	0.40
1:E:425:ILE:HG12	1:E:442:LEU:HD12	2.03	0.40
1:E:700:SER:HB2	1:E:743:TYR:CE1	2.56	0.40
1:A:306:ASP:OD1	1:A:377:GLN:HG2	2.21	0.40
1:A:795:SER:OG	1:A:797:ASN:OD1	2.39	0.40
1:A:820:LEU:HA	1:A:823:ILE:HG13	2.03	0.40
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.78	0.40
1:B:942:PHE:O	1:B:946:PRO:HB3	2.21	0.40
2:C:65:ASN:OD1	2:C:66:ALA:N	2.54	0.40
1:D:610:GLN:HG3	1:D:614:ASN:HD21	1.87	0.40
1:D:619:LEU:HD23	1:D:619:LEU:HA	1.89	0.40
1:E:222:ASP:OD1	1:E:223:TYR:N	2.54	0.40
1:E:359:ARG:NH1	1:E:363:LEU:HD12	2.37	0.40
1:E:985:LYS:O	1:E:988:VAL:HG12	2.21	0.40
1:A:90:ILE:O	1:A:94:VAL:HB	2.21	0.40
1:A:253:ILE:HD12	1:A:253:ILE:HA	1.89	0.40
1:A:819:ARG:HA	1:A:822:GLU:CD	2.46	0.40
1:A:841:LEU:HB3	1:A:844:LEU:HD23	2.03	0.40
1:B:310:ASP:OD1	1:B:380:ARG:NH2	2.55	0.40
1:B:498:LEU:HD21	2:C:23:PHE:CE2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LYS:HE2	1:D:231:TRP:CD1	2.56	0.40
1:D:282:TYR:O	1:D:285:ARG:HG3	2.21	0.40
1:D:737:VAL:HG13	1:D:758:LEU:HD21	2.03	0.40
1:E:82:ASP:OD1	1:E:83:GLU:HG3	2.21	0.40
1:A:67:HIS:CE1	1:A:71:TYR:HD2	2.39	0.40
1:A:155:GLU:OE1	1:A:199:LEU:HB2	2.21	0.40
1:A:609:HIS:ND1	1:A:658:HIS:HD2	2.19	0.40
1:A:682:GLU:O	1:A:685:GLU:HG2	2.21	0.40
1:B:957:SER:HA	1:B:960:LYS:HG2	2.03	0.40
2:C:176:ARG:HD3	2:C:192:TYR:CD2	2.56	0.40
1:D:115:ASN:HB2	1:D:116:PRO:HD2	2.04	0.40
1:D:116:PRO:HA	1:D:119:ASP:OD2	2.22	0.40
1:D:418:TYR:HA	1:D:421:MET:CE	2.51	0.40
1:D:549:GLN:H	1:D:549:GLN:HG3	1.64	0.40
1:E:312:ILE:HG21	1:E:360:PHE:CE2	2.57	0.40
1:A:89:GLN:HE22	1:A:188:ASP:CG	2.29	0.40
1:A:244:PHE:CD1	1:A:267:ARG:HB3	2.57	0.40
1:A:612:ILE:HG21	1:A:658:HIS:CG	2.56	0.40
1:A:995:ARG:HE	1:A:999:ILE:HG13	1.87	0.40
1:B:934:ILE:HD11	1:B:945:ASP:OD2	2.22	0.40
1:D:144:LYS:HB2	1:D:144:LYS:HE2	1.86	0.40
1:D:215:PHE:HB2	1:D:245:PHE:HA	2.02	0.40
1:D:720:LEU:HB3	1:D:757:TRP:CD1	2.57	0.40
1:D:959:LEU:HA	1:D:962:TYR:CD2	2.55	0.40
1:E:312:ILE:HD12	1:E:334:PHE:HE2	1.86	0.40
1:E:361:PHE:HB2	1:E:396:MET:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	893/1005 (89%)	861 (96%)	32 (4%)	0	100	100
1	B	903/1005 (90%)	874 (97%)	29 (3%)	0	100	100
1	D	901/1005 (90%)	878 (97%)	23 (3%)	0	100	100
1	E	899/1005 (90%)	864 (96%)	35 (4%)	0	100	100
2	C	106/264 (40%)	96 (91%)	10 (9%)	0	100	100
2	F	106/264 (40%)	104 (98%)	2 (2%)	0	100	100
All	All	3808/4548 (84%)	3677 (97%)	131 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	844/923 (91%)	829 (98%)	15 (2%)	51	65
1	B	849/923 (92%)	835 (98%)	14 (2%)	55	66
1	D	849/923 (92%)	835 (98%)	14 (2%)	55	66
1	E	846/923 (92%)	833 (98%)	13 (2%)	57	66
2	C	102/225 (45%)	98 (96%)	4 (4%)	28	51
2	F	102/225 (45%)	102 (100%)	0	100	100
All	All	3592/4142 (87%)	3532 (98%)	60 (2%)	52	65

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	104	LEU
1	A	114	THR
1	A	131	THR
1	A	183	VAL
1	A	213	ILE
1	A	293	LEU

Continued on next page...

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Mol	Chain	Res	Type
1	A	347	VAL
1	A	366	SER
1	A	697	LYS
1	A	740	LEU
1	A	748	ASP
1	A	822	GLU
1	A	852	HIS
1	A	938	ASP
1	B	85	LEU
1	B	160	ASN
1	B	274	LEU
1	B	379	GLU
1	B	520	THR
1	B	553	ASP
1	B	671	CYS
1	B	714	SER
1	B	726	VAL
1	B	757	TRP
1	B	782	GLN
1	B	835	ILE
1	B	859	VAL
1	B	926	ASN
2	C	8	THR
2	C	173	VAL
2	C	192	TYR
2	C	198	VAL
1	D	131	THR
1	D	134	TYR
1	D	207	ILE
1	D	222	ASP
1	D	257	THR
1	D	322	LEU
1	D	455	TYR
1	D	484	SER
1	D	507	PHE
1	D	549	GLN
1	D	607	GLU
1	D	654	ASN
1	D	824	THR
1	D	993	ASP
1	E	114	THR
1	E	119	ASP

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Mol	Chain	Res	Type
1	E	134	TYR
1	E	213	ILE
1	E	378	TYR
1	E	419	ASP
1	E	498	LEU
1	E	554	ASP
1	E	590	ASP
1	E	600	LEU
1	E	778	PHE
1	E	810	HIS
1	E	885	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	351	ASN
1	A	483	GLN
1	A	493	ASN
1	A	536	GLN
1	A	563	ASN
1	A	654	ASN
1	A	658	HIS
1	A	681	GLN
1	A	786	HIS
1	A	852	HIS
1	A	895	ASN
1	A	939	GLN
1	A	973	ASN
1	B	263	ASN
1	B	461	ASN
1	B	503	HIS
1	B	521	ASN
1	B	702	ASN
1	B	786	HIS
1	B	867	ASN
2	C	34	GLN
2	C	194	GLN
1	D	475	GLN
1	D	477	ASN
1	D	591	ASN
1	D	610	GLN

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Mol	Chain	Res	Type
1	D	614	ASN
1	D	658	HIS
1	D	705	ASN
1	D	765	ASN
1	D	829	GLN
1	D	867	ASN
1	D	973	ASN
1	E	263	ASN
1	E	339	HIS
1	E	377	GLN
1	E	391	ASN
1	E	428	GLN
1	E	814	ASN
1	E	832	GLN
1	E	834	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

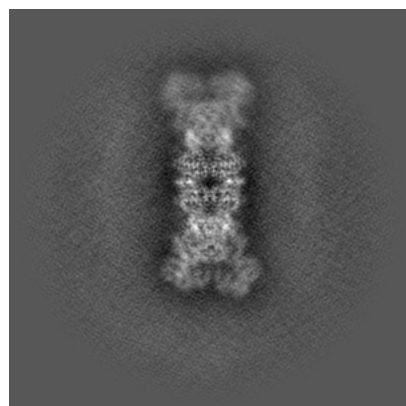
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37921. These allow visual inspection of the internal detail of the map and identification of artifacts.

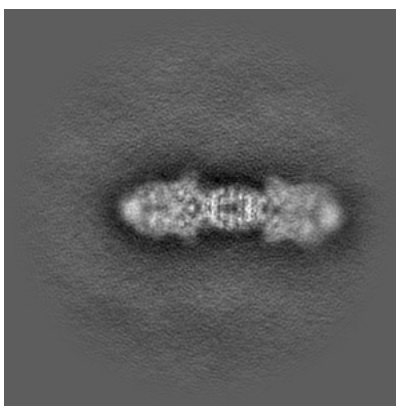
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

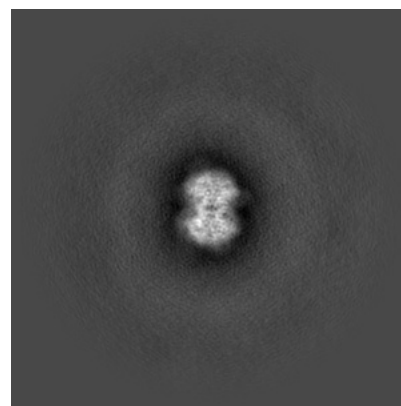
6.1.1 Primary map



X

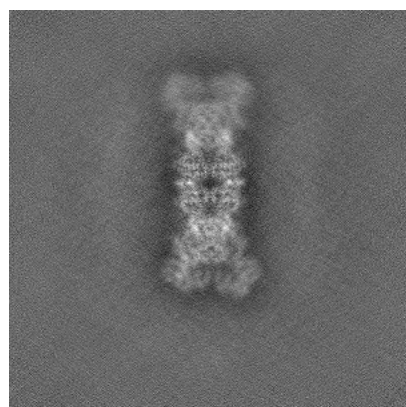


Y

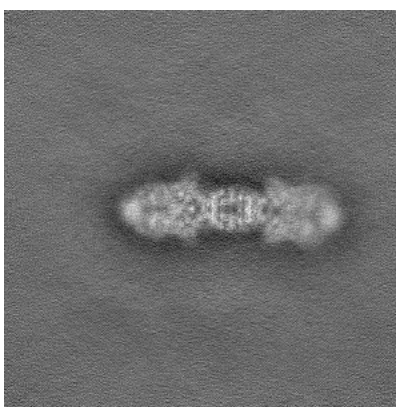


Z

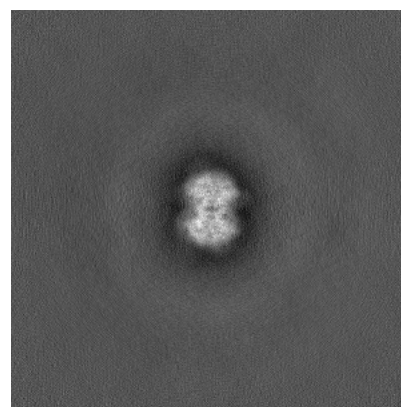
6.1.2 Raw map



X



Y

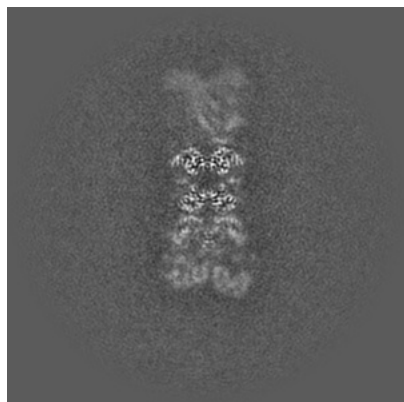


Z

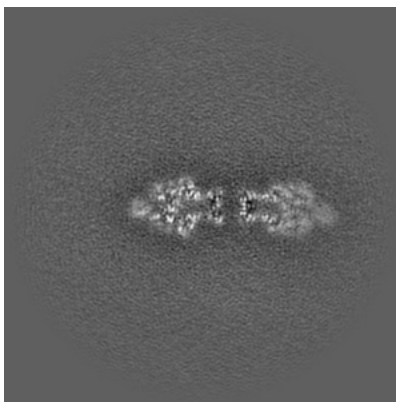
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

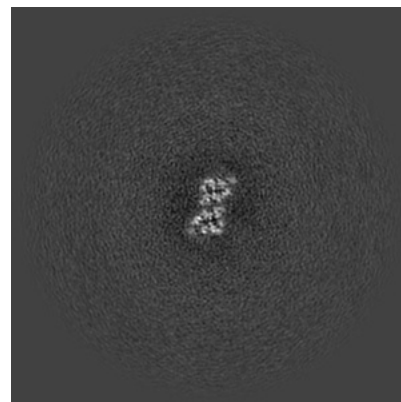
6.2.1 Primary map



X Index: 230

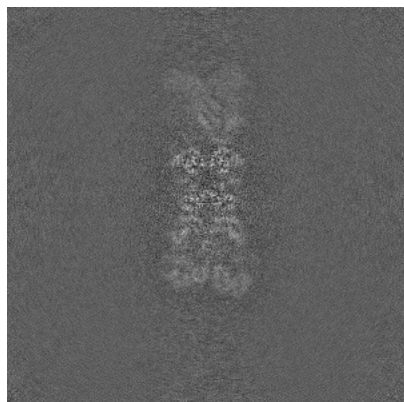


Y Index: 230



Z Index: 230

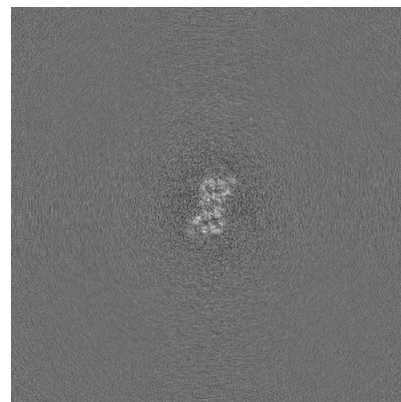
6.2.2 Raw map



X Index: 230



Y Index: 230

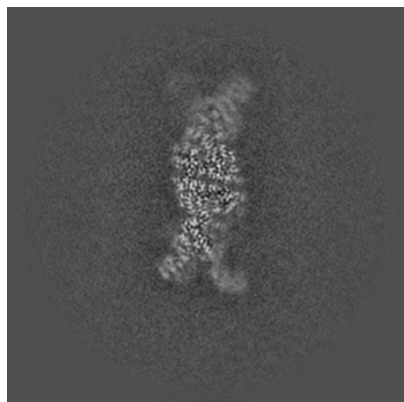


Z Index: 230

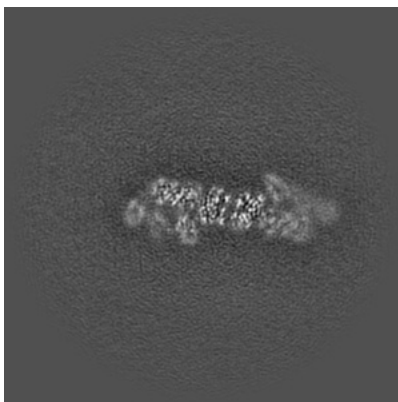
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

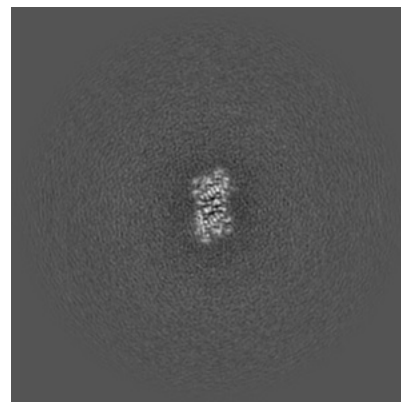
6.3.1 Primary map



X Index: 241

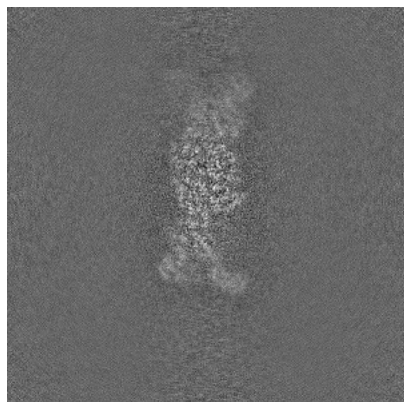


Y Index: 217

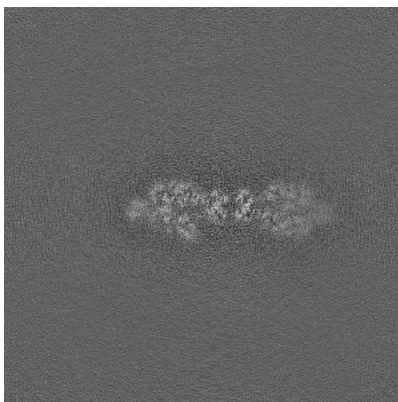


Z Index: 240

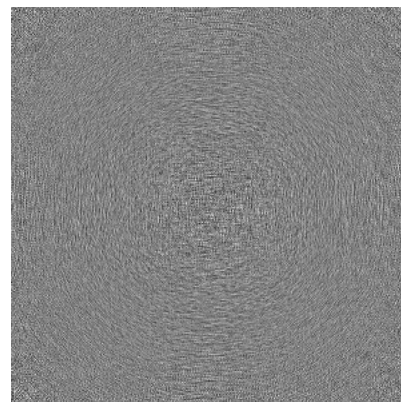
6.3.2 Raw map



X Index: 239



Y Index: 226

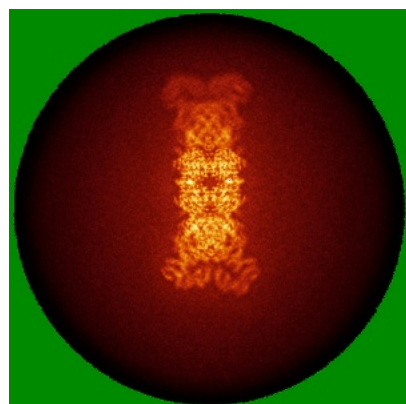


Z Index: 459

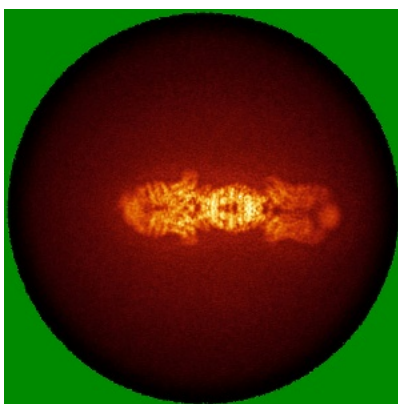
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

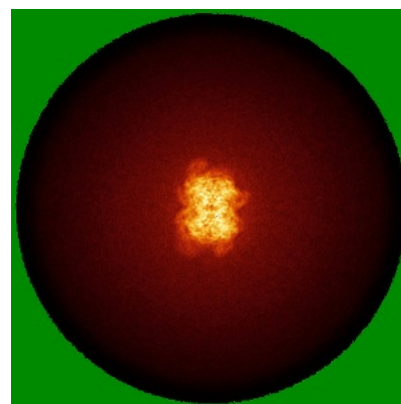
6.4.1 Primary map



X

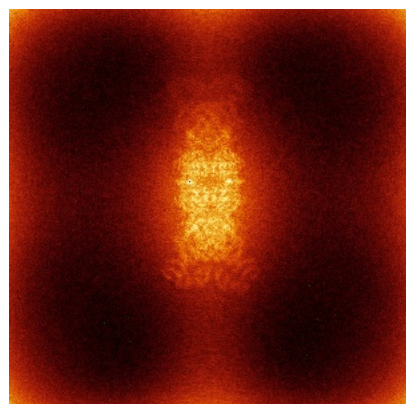


Y

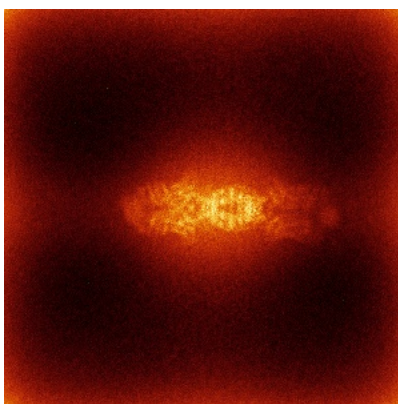


Z

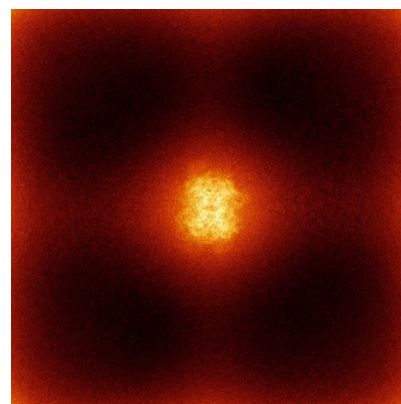
6.4.2 Raw map



X



Y

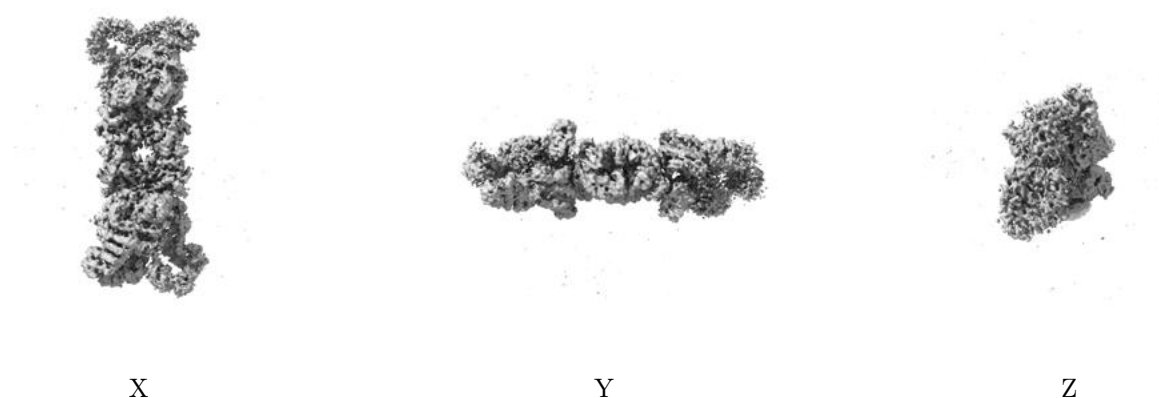


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

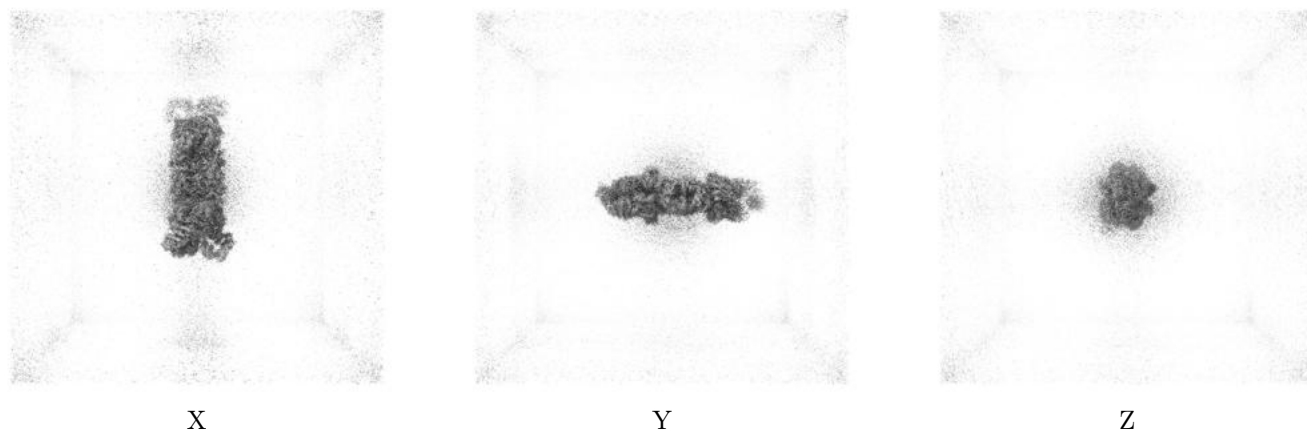
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

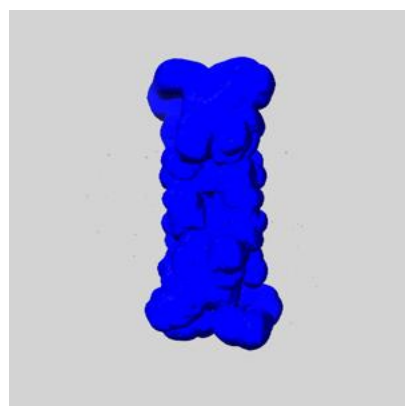
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

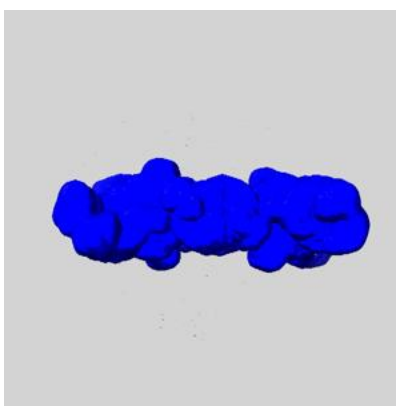
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

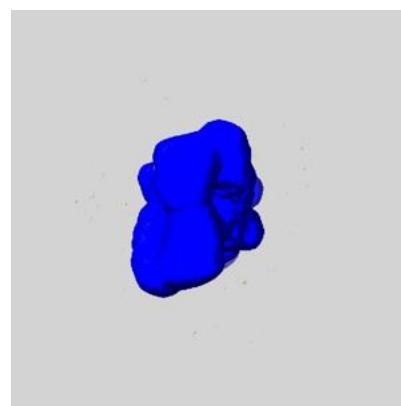
6.6.1 emd_37921_msk_1.map [i](#)



X



Y

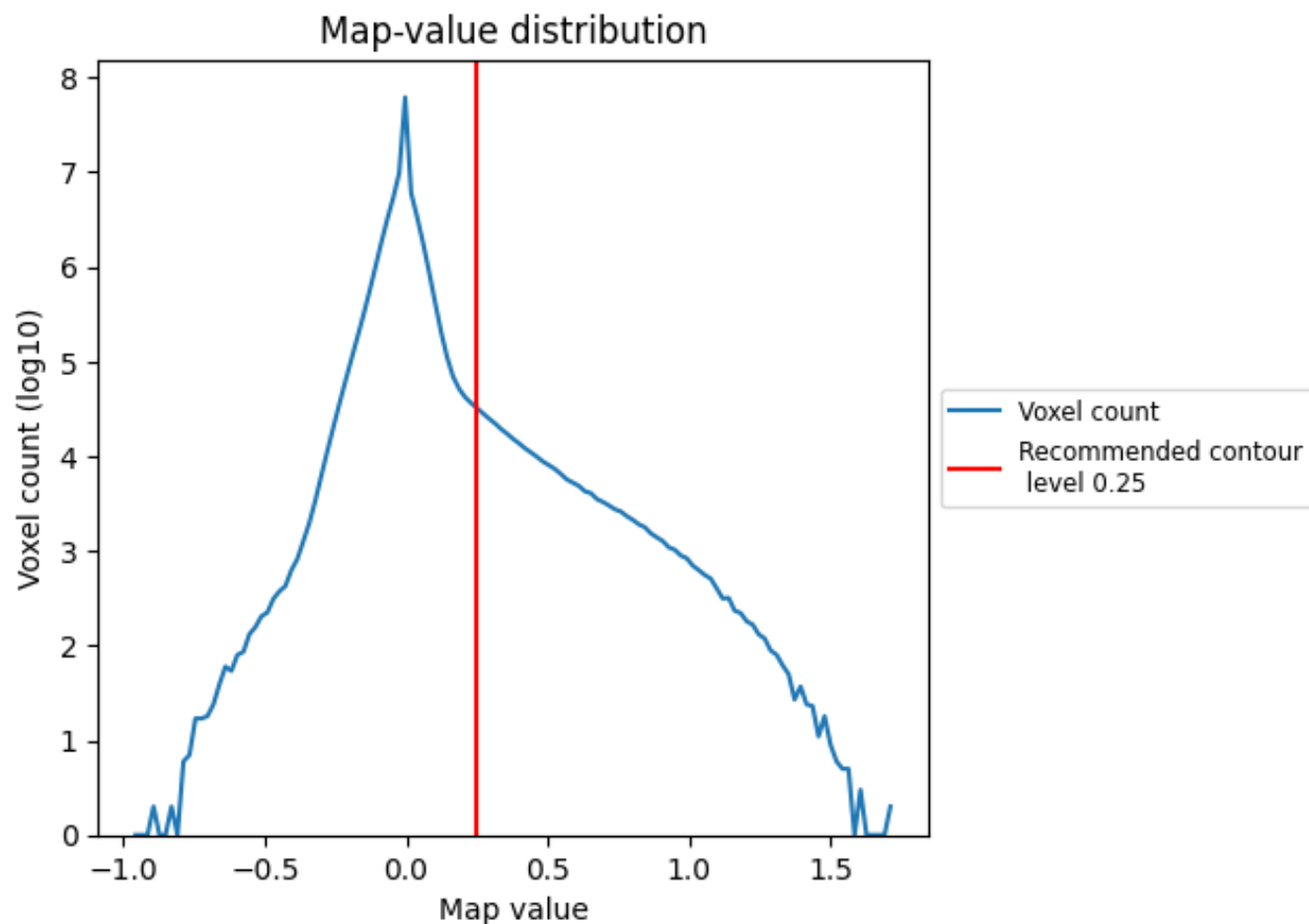


Z

7 Map analysis [i](#)

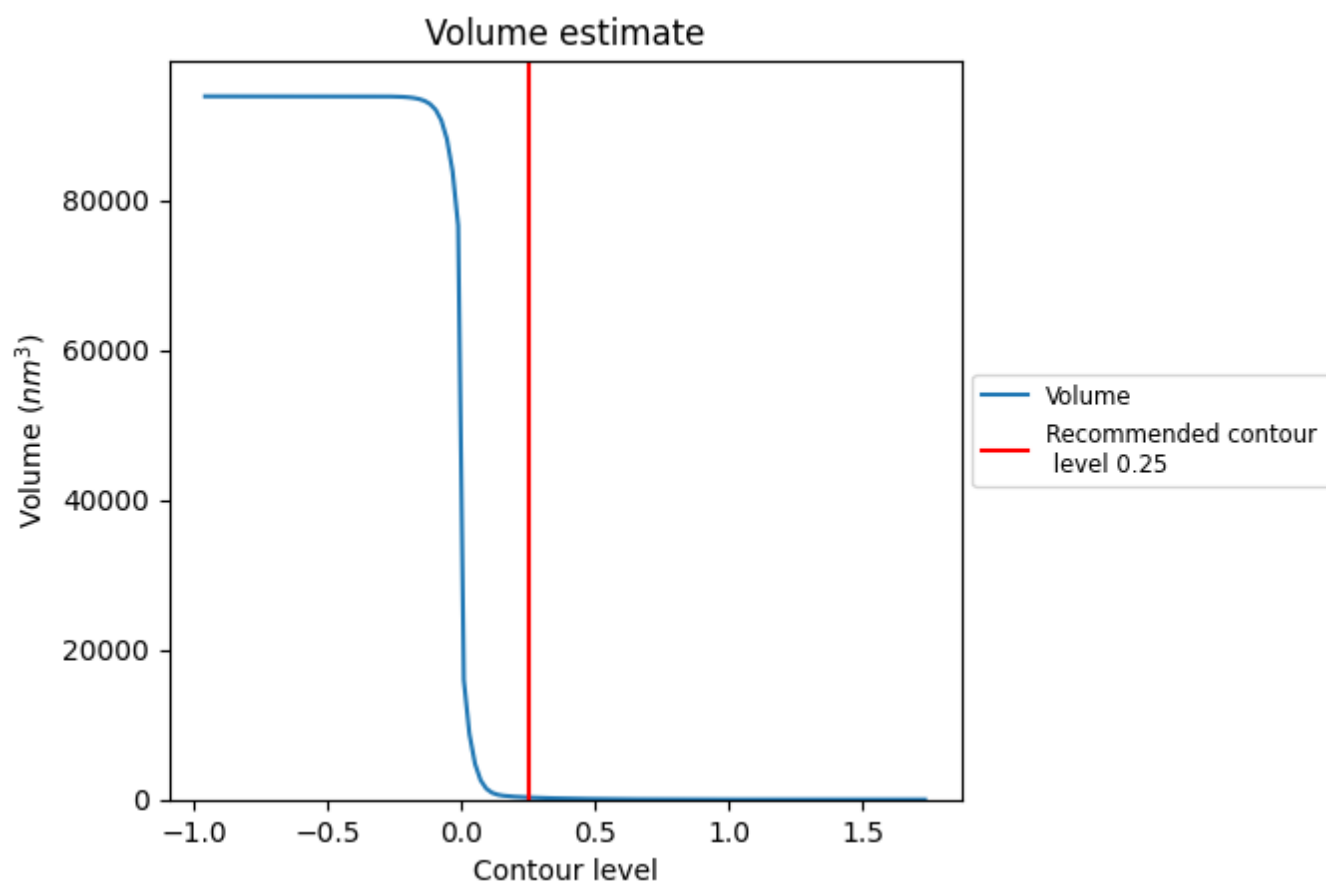
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

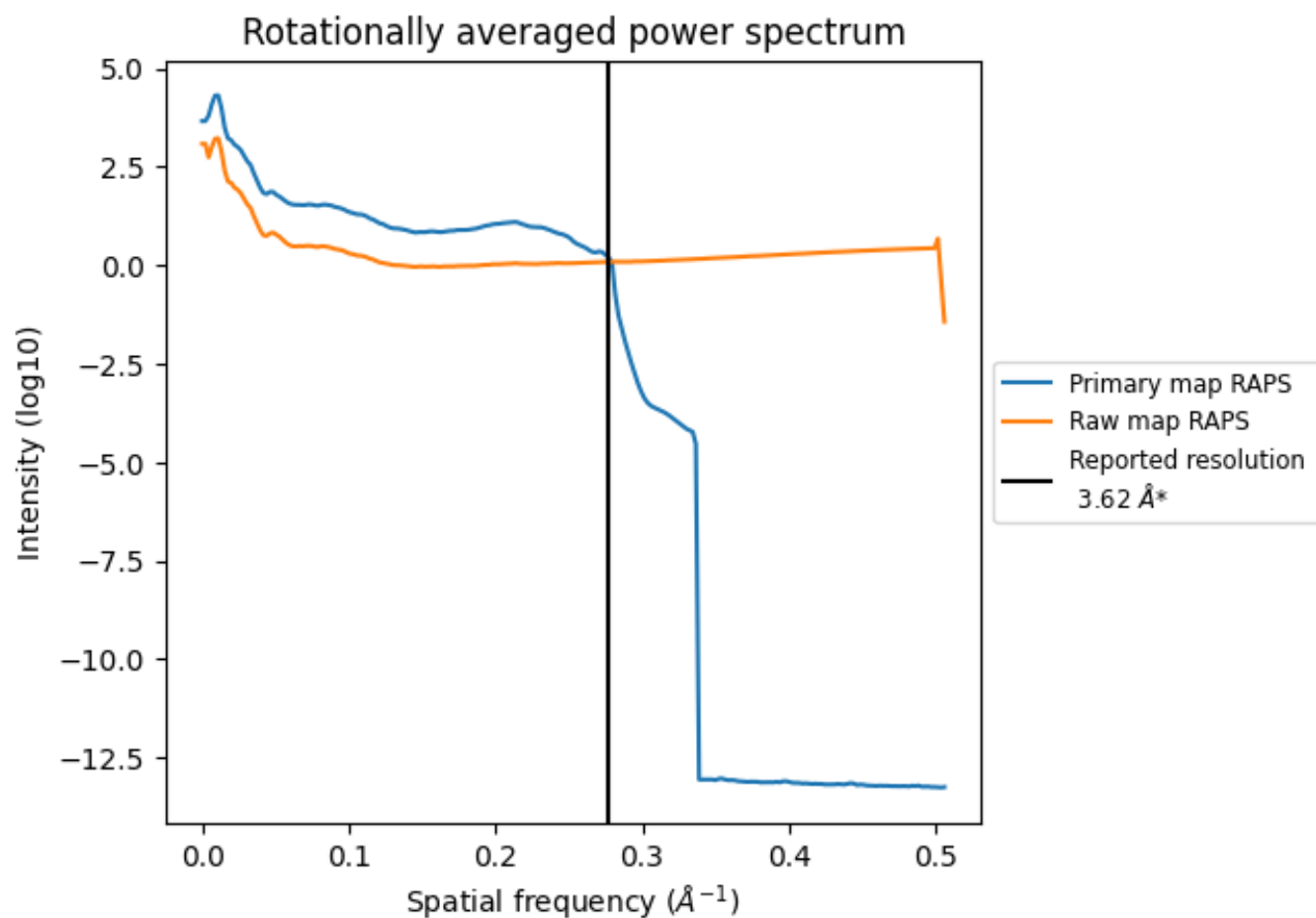
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 288 nm³; this corresponds to an approximate mass of 260 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

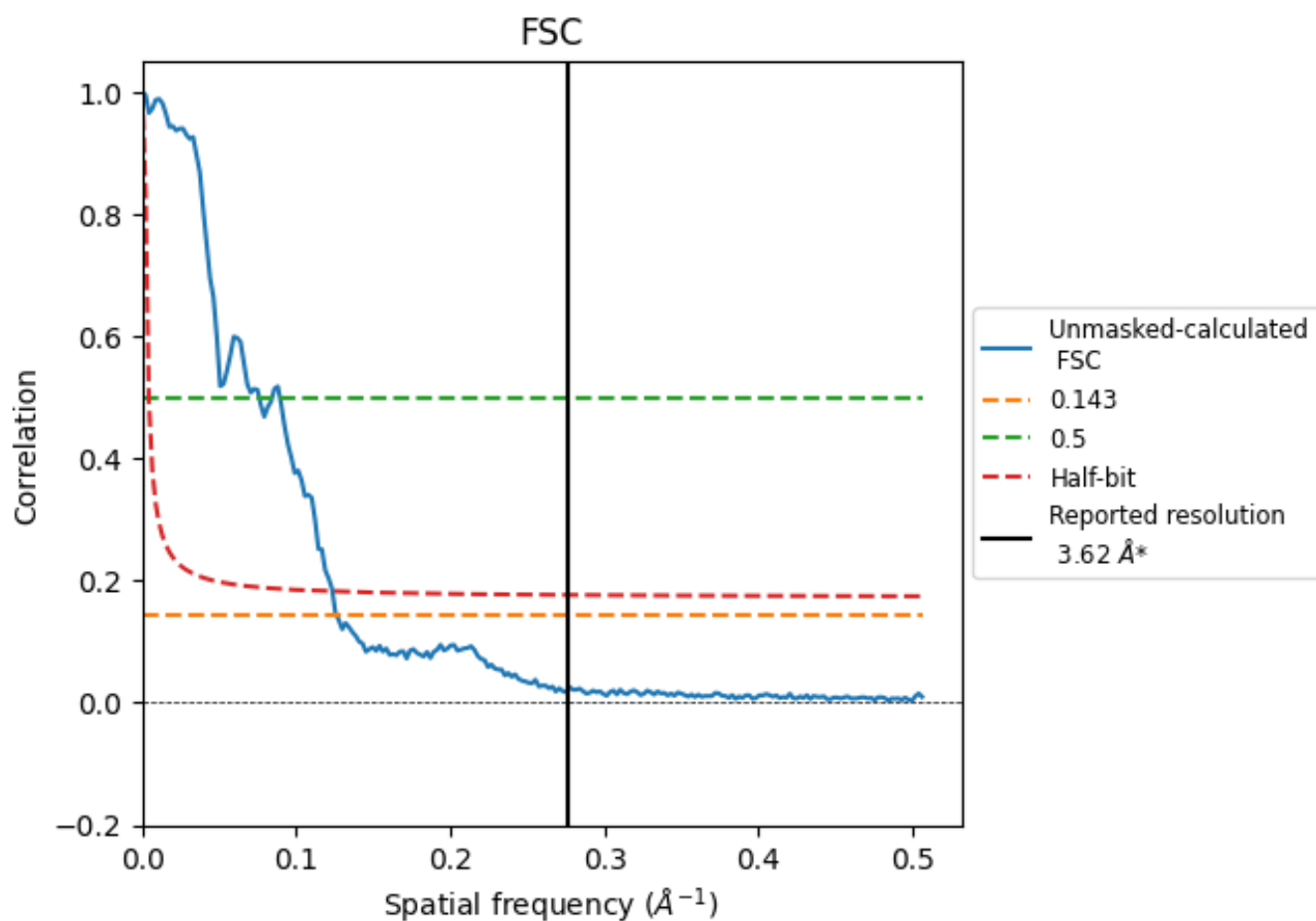


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

8.2 Resolution estimates [i](#)

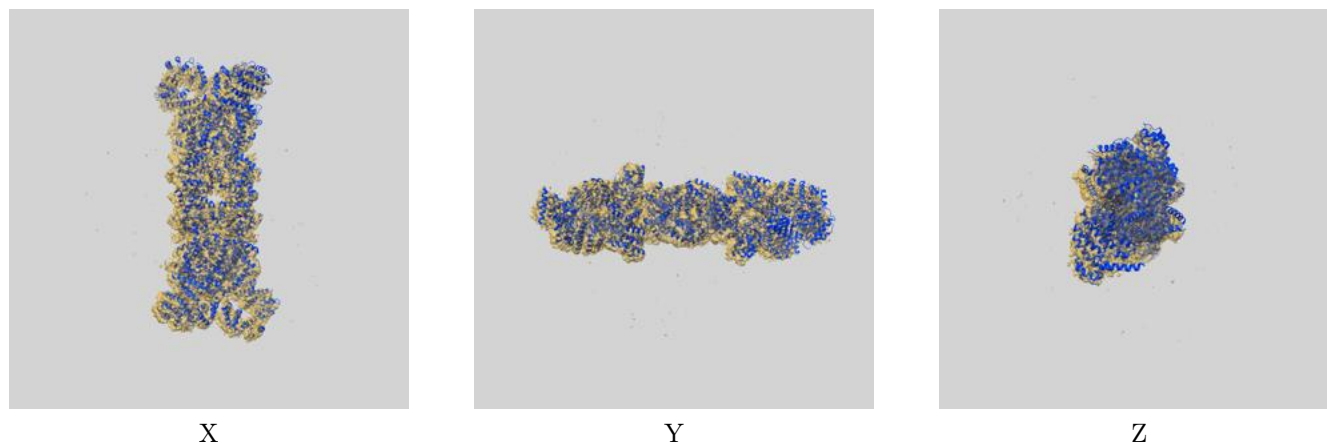
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.93	13.18	8.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.93 differs from the reported value 3.62 by more than 10 %

9 Map-model fit [i](#)

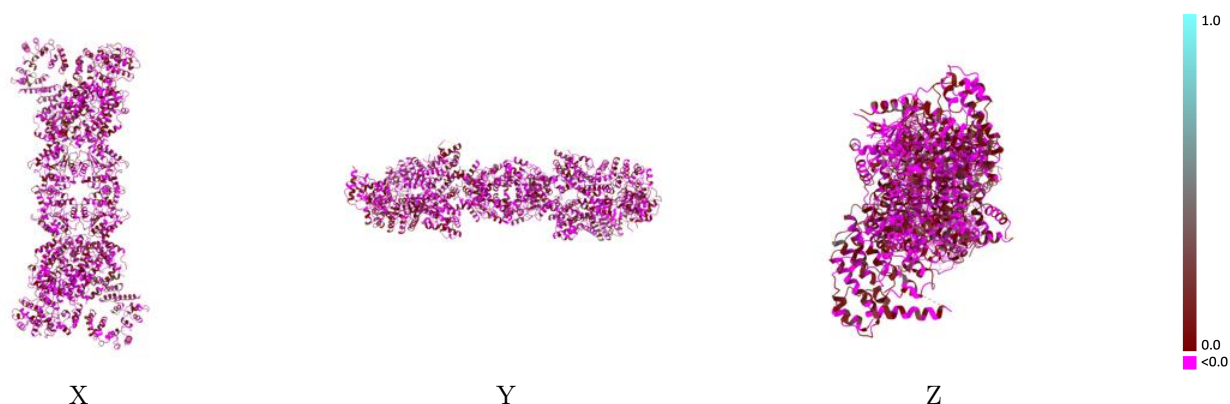
This section contains information regarding the fit between EMDB map EMD-37921 and PDB model 8WYA. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



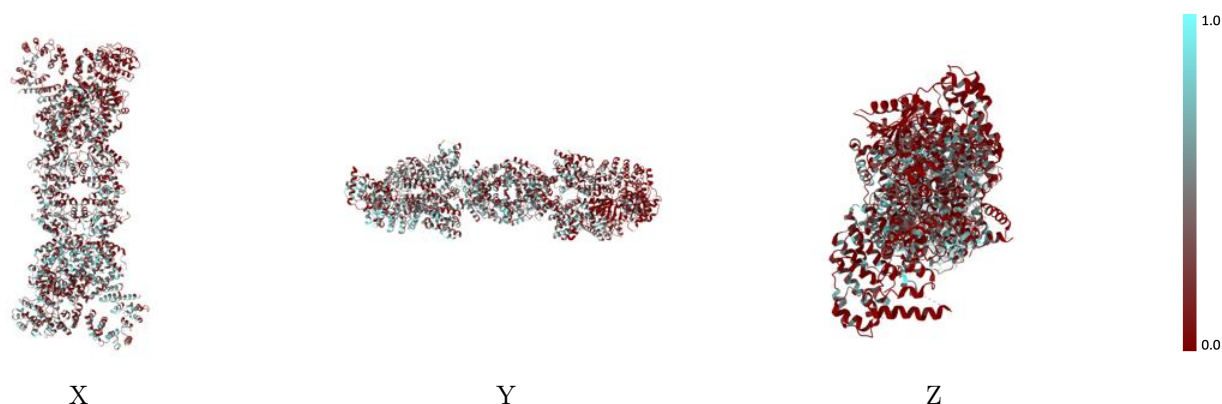
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



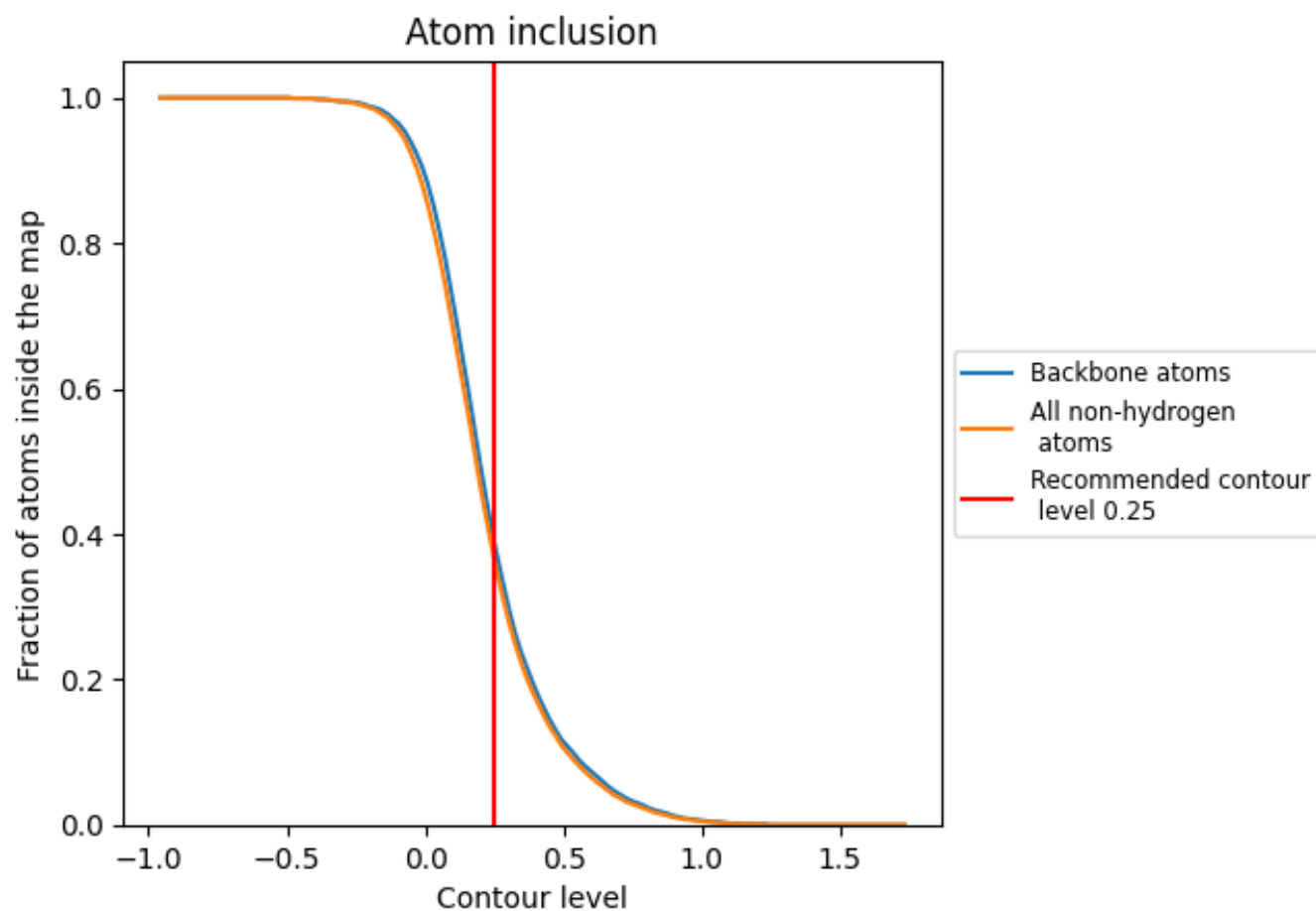
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3640	0.0110
A	0.4410	0.0090
B	0.4560	0.0130
C	0.2300	-0.0050
D	0.3100	0.0190
E	0.3070	0.0110
F	0.0240	-0.0250

1.0
0.0
-0.0